



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:12 PM UTC

PDB ID : 4S13 / pdb_00004s13
Title : Ferulic Acid Decarboxylase (FDC1)
Authors : Lee, S.G.; Bhuiya, M.W.; Yu, O.; Jez, J.M.
Deposited on : 2015-01-07
Resolution : 2.35 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

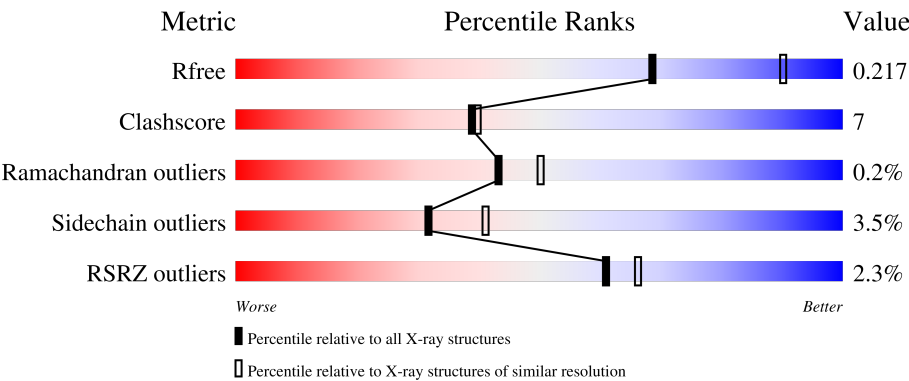
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	503	82%12%6%
1	B	503	81%12%5%
1	C	503	81%17%
1	D	503	82%12%5%
1	E	503	83%14%

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Mol	Chain	Length	Quality of chain
1	F	503	2% 79% 19%
1	G	503	4% 75% 16% • 6%
1	H	503	5% 77% 17% • •

2 Entry composition

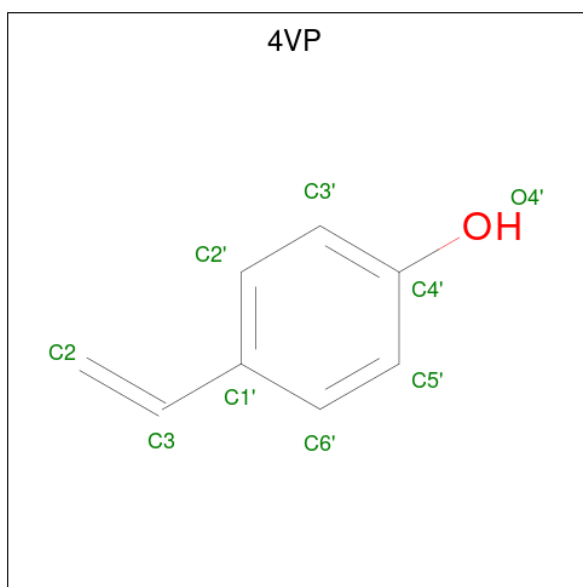
There are 3 unique types of molecules in this entry. The entry contains 31691 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferulic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3705	2387	600	696	22			
1	B	476	Total	C	N	O	S	0	2	0
			3748	2420	604	701	23			
1	C	501	Total	C	N	O	S	0	0	0
			3933	2536	642	733	22			
1	D	480	Total	C	N	O	S	0	1	0
			3775	2436	610	707	22			
1	E	492	Total	C	N	O	S	0	0	0
			3868	2495	630	721	22			
1	F	501	Total	C	N	O	S	0	0	0
			3933	2536	642	733	22			
1	G	472	Total	C	N	O	S	0	1	0
			3718	2399	600	697	22			
1	H	481	Total	C	N	O	S	0	1	0
			3777	2435	611	709	22			

- Molecule 2 is 4-ethenylphenol (CCD ID: 4VP) (formula: C₈H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	8	1		
2	C	1	Total	C	O	0	0
			9	8	1		
2	E	1	Total	C	O	0	0
			9	8	1		
2	F	1	Total	C	O	0	0
			9	8	1		
2	G	1	Total	C	O	0	0
			9	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	190	Total	O	0	0
			190	190		
3	C	131	Total	O	0	0
			131	131		
3	D	185	Total	O	0	0
			185	185		
3	E	165	Total	O	0	0
			165	165		
3	F	137	Total	O	0	0
			137	137		
3	G	100	Total	O	0	0
			100	100		

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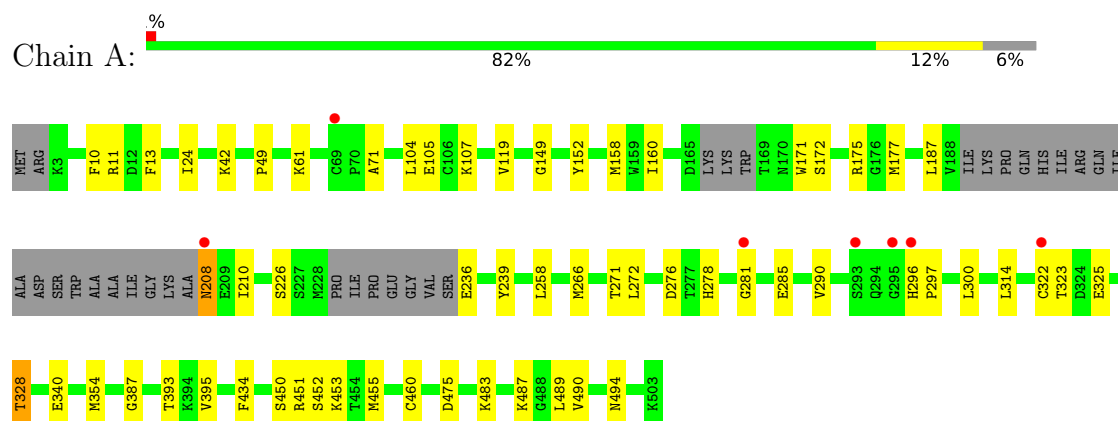
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	129	Total 129	O 129	0	0

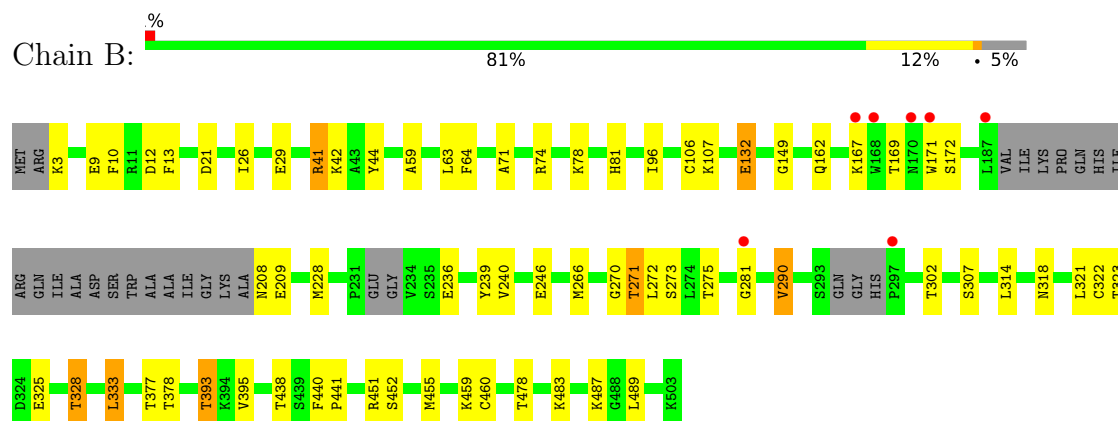
3 Residue-property plots

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.

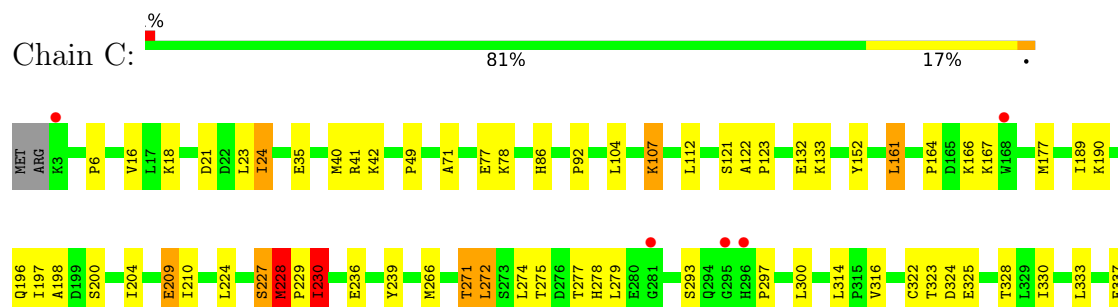
• Molecule 1: Ferulic acid decarboxylase 1

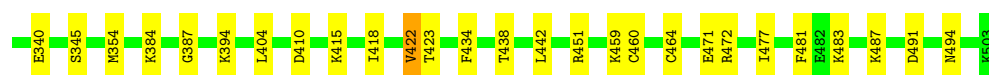


• Molecule 1: Ferulic acid decarboxylase 1

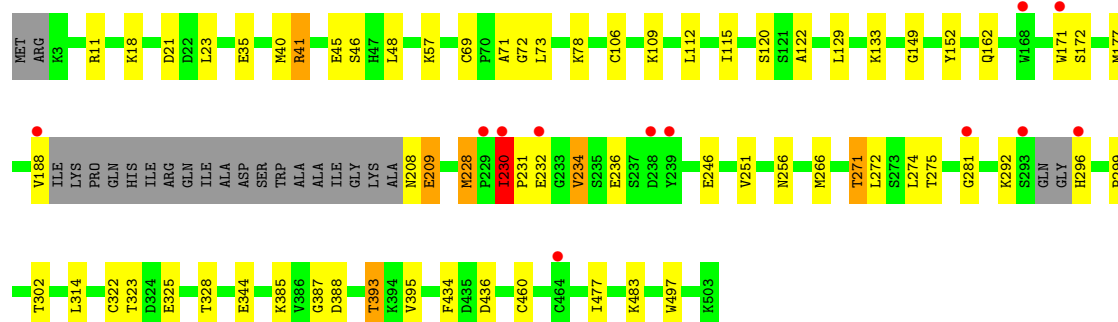
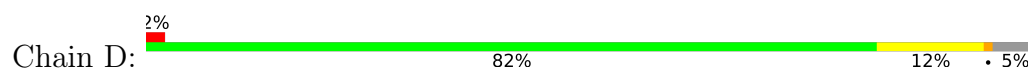


• Molecule 1: Ferulic acid decarboxylase 1

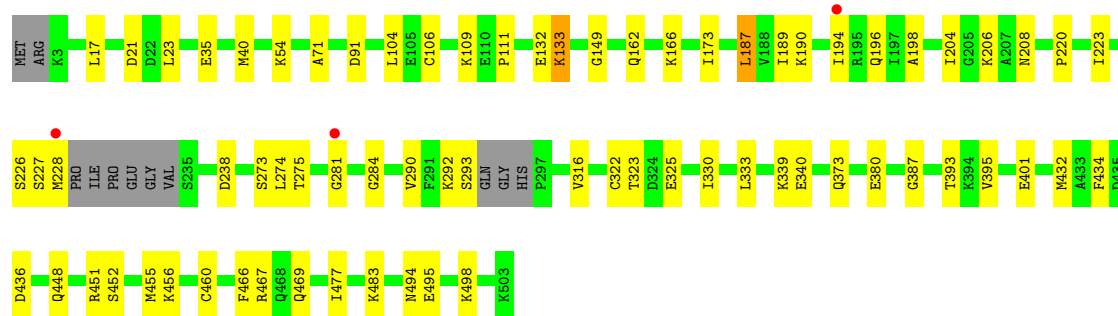
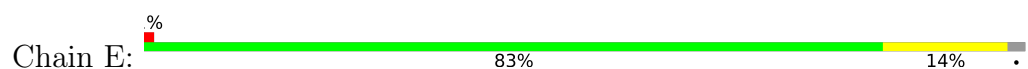




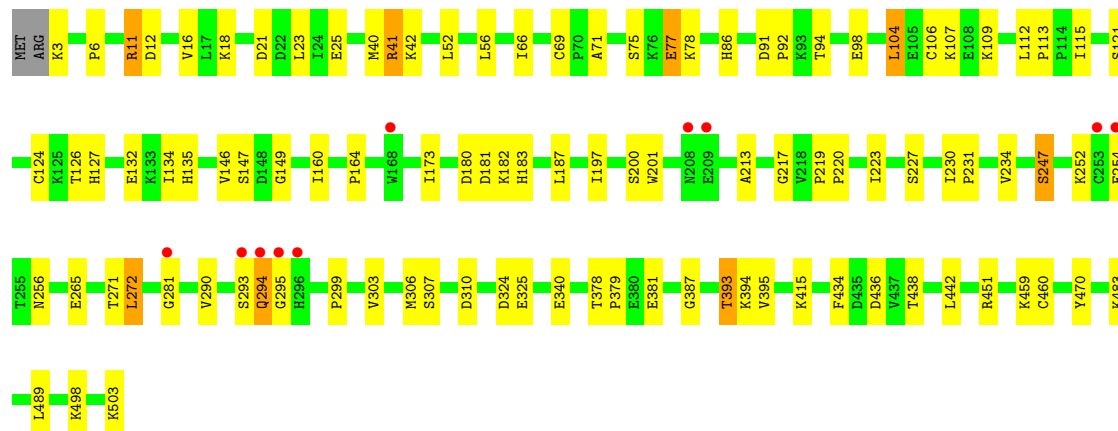
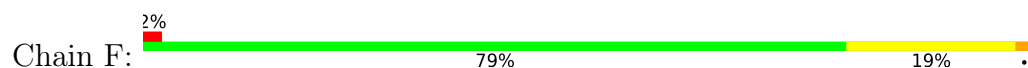
• Molecule 1: Ferulic acid decarboxylase 1



• Molecule 1: Ferulic acid decarboxylase 1

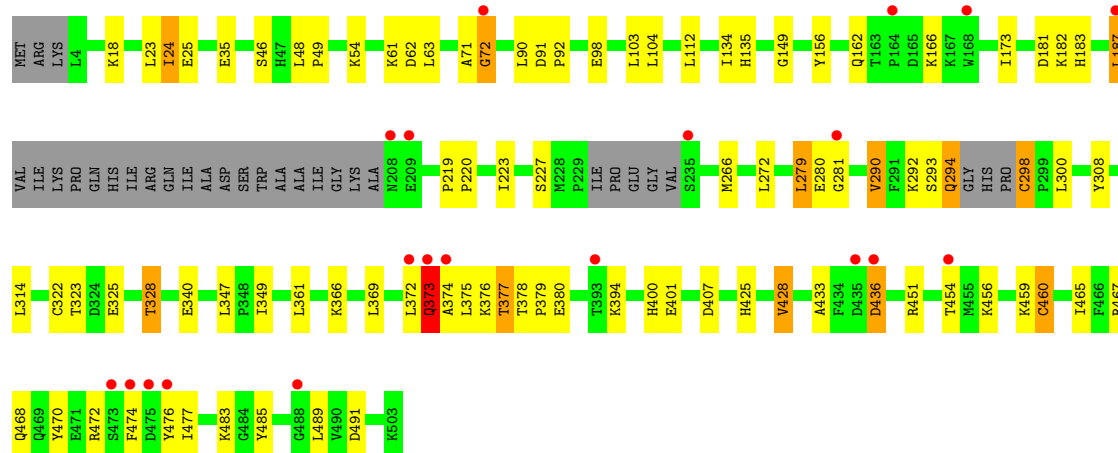


• Molecule 1: Ferulic acid decarboxylase 1



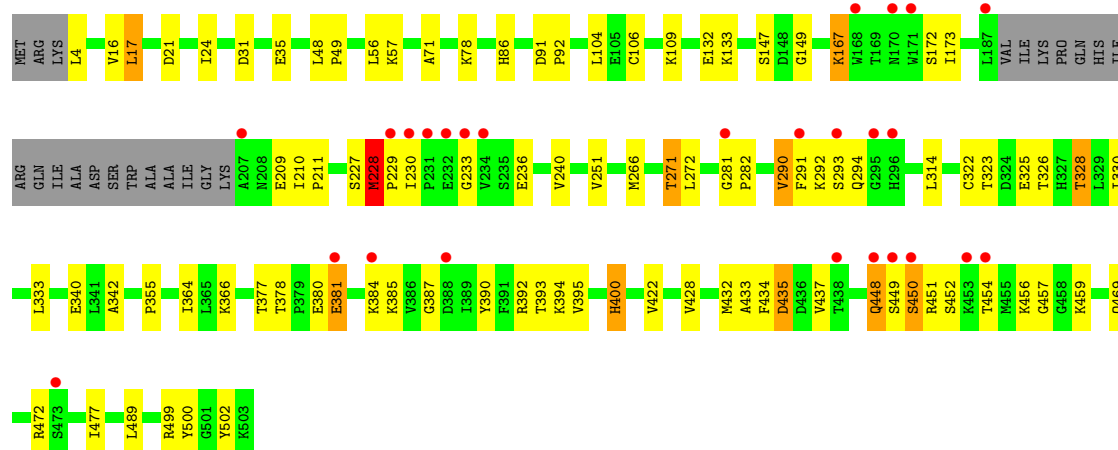
• Molecule 1: Ferulic acid decarboxylase 1

Chain G: 4% 75% 16% 6%



• Molecule 1: Ferulic acid decarboxylase 1

Chain H: 5% 77% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	251.96Å 121.00Å 159.56Å 90.00° 121.93° 90.00°	Depositor
Resolution (Å)	47.05 – 2.35 47.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.8 (47.05-2.35) 91.5 (47.05-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.171 , 0.215 0.174 , 0.217	Depositor DCC
R_{free} test set	8159 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtrriage
Anisotropy	0.566	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31691	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.96 % 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 9.2052e-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: 4VP

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	0.57	0/3794	0.83	0/5147
1	B	0.57	0/3846	0.84	2/5218 (0.0%)
1	C	0.54	0/4033	0.83	6/5477 (0.1%)
1	D	0.59	0/3872	0.83	5/5256 (0.1%)
1	E	0.54	0/3963	0.81	2/5376 (0.0%)
1	F	0.54	0/4033	0.84	4/5477 (0.1%)
1	G	0.50	0/3811	0.84	5/5170 (0.1%)
1	H	0.54	0/3875	0.85	0/5262
All	All	0.55	0/31227	0.83	24/42383 (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	C	0	1
1	G	0	3
1	H	0	1
All	All	0	5

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	LEU	CA-C-N	8.11	125.58	119.66
1	C	112	LEU	C-N-CA	8.11	125.58	119.66
1	G	374	ALA	N-CA-C	-7.15	103.82	112.54
1	D	228	MET	CA-C-N	6.80	128.34	119.84
1	D	228	MET	C-N-CA	6.80	128.34	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	112	LEU	CA-C-N	6.33	124.22	119.66
1	G	112	LEU	C-N-CA	6.33	124.22	119.66
1	E	91	ASP	CA-C-N	6.00	125.68	119.56
1	E	91	ASP	C-N-CA	6.00	125.68	119.56
1	C	122	ALA	CA-C-N	5.59	125.95	119.47
1	C	122	ALA	C-N-CA	5.59	125.95	119.47
1	C	230	ILE	CA-C-N	5.42	126.61	119.84
1	C	230	ILE	C-N-CA	5.42	126.61	119.84
1	G	219	PRO	CA-C-N	5.33	125.66	119.47
1	G	219	PRO	C-N-CA	5.33	125.66	119.47
1	F	219	PRO	CA-C-N	5.33	126.50	119.84
1	F	219	PRO	C-N-CA	5.33	126.50	119.84
1	F	91	ASP	CA-C-N	5.22	125.53	119.47
1	F	91	ASP	C-N-CA	5.22	125.53	119.47
1	D	122	ALA	CA-C-N	5.13	125.17	119.32
1	D	122	ALA	C-N-CA	5.13	125.17	119.32
1	B	487	LYS	CA-C-N	-5.04	117.44	123.44
1	B	487	LYS	C-N-CA	-5.04	117.44	123.44
1	D	73	LEU	N-CA-C	5.02	117.94	110.52

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	228	MET	Peptide
1	G	373	GLN	Peptide
1	G	476	TYR	Peptide
1	G	72	GLY	Peptide
1	H	228	MET	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	3705	0	3702	40	0
1	B	3748	0	3761	47	0
1	C	3933	0	3944	55	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3775	0	3781	39	0
1	E	3868	0	3882	45	0
1	F	3933	0	3944	63	0
1	G	3718	0	3722	70	1
1	H	3777	0	3776	74	0
2	A	9	0	8	2	0
2	C	9	0	8	2	0
2	E	9	0	8	1	0
2	F	9	0	8	0	0
2	G	9	0	8	0	0
3	A	152	0	0	9	0
3	B	190	0	0	9	0
3	C	131	0	0	6	0
3	D	185	0	0	12	0
3	E	165	0	0	10	0
3	F	137	0	0	8	0
3	G	100	0	0	7	0
3	H	129	0	0	10	0
All	All	31691	0	30552	412	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 7.

All (412) 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:D:208:ASN:N	3:D:762:HOH:O	1.93	1.00
1:C:410:ASP:OD2	3:C:736:HOH:O	1.82	0.95
1:G:24[B]:ILE:HD11	1:G:49:PRO:HB2	1.55	0.88
1:C:228:MET:HB3	1:C:229:PRO:HD3	1.55	0.88
1:D:296:HIS:N	3:D:760:HOH:O	2.05	0.88
1:G:90:LEU:O	3:G:726:HOH:O	1.89	0.88
1:D:292:LYS:O	3:D:754:HOH:O	1.90	0.87
1:F:294:GLN:OE1	3:F:825:HOH:O	1.96	0.84
1:B:290:VAL:HG13	1:E:477:ILE:HB	1.59	0.83
1:D:71:ALA:HB3	1:D:325:GLU:HG3	1.57	0.83
1:G:394:LYS:NZ	3:G:778:HOH:O	2.11	0.82
1:B:41:ARG:NH1	1:B:318:ASN:O	2.15	0.79
1:B:41:ARG:NH2	1:B:321:LEU:O	2.16	0.78
1:E:330:ILE:HD13	2:E:601:4VP:H4	1.66	0.78
1:C:198:ALA:HB1	1:C:274:LEU:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:503:LYS:O	3:F:780:HOH:O	2.01	0.77
1:G:71:ALA:HB3	1:G:325:GLU:HG3	1.67	0.77
1:B:59:ALA:O	3:B:701:HOH:O	2.01	0.76
1:B:71:ALA:HB3	1:B:325:GLU:HG3	1.66	0.76
1:G:290:VAL:HG13	1:H:477:ILE:HB	1.65	0.76
1:D:388:ASP:OD2	3:D:731:HOH:O	2.02	0.76
1:H:366:LYS:NZ	3:H:728:HOH:O	2.11	0.76
1:B:29:GLU:O	3:B:694:HOH:O	2.02	0.76
1:A:105:GLU:OE1	3:A:744:HOH:O	2.04	0.75
1:F:135:HIS:ND1	1:F:181:ASP:OD2	2.20	0.75
1:C:71:ALA:HB3	1:C:325:GLU:HG3	1.68	0.74
1:F:113:PRO:O	1:F:247:SER:OG	2.04	0.74
1:F:393:THR:HG22	1:F:395:VAL:H	1.53	0.74
1:E:71:ALA:HB3	1:E:325:GLU:HG3	1.69	0.73
1:F:378:THR:OG1	1:F:381:GLU:OE1	2.05	0.73
1:G:477:ILE:HB	1:H:290:VAL:HG13	1.70	0.73
1:F:503:LYS:NZ	3:F:815:HOH:O	2.19	0.73
1:H:435:ASP:N	1:H:435:ASP:OD1	2.22	0.73
1:A:475:ASP:OD1	3:A:788:HOH:O	2.06	0.72
1:E:292:LYS:O	3:E:831:HOH:O	2.06	0.72
1:C:487:LYS:NZ	1:C:491:ASP:OD1	2.20	0.72
1:H:381:GLU:N	3:H:726:HOH:O	2.20	0.72
1:F:436:ASP:OD2	3:F:771:HOH:O	2.07	0.71
1:H:133:LYS:NZ	3:H:690:HOH:O	2.16	0.71
1:F:11:ARG:NH2	1:F:265:GLU:OE2	2.23	0.71
1:H:71:ALA:HB3	1:H:325:GLU:HG3	1.71	0.71
1:A:393:THR:HG22	1:A:395:VAL:H	1.55	0.70
1:A:171:TRP:HB2	1:A:236:GLU:HG3	1.73	0.70
1:D:230:ILE:HG12	1:D:231:PRO:HD2	1.72	0.70
1:D:120:SER:OG	3:D:649:HOH:O	1.95	0.69
1:B:393:THR:HG22	1:B:395:VAL:H	1.56	0.69
1:D:11:ARG:NH1	3:D:738:HOH:O	2.08	0.69
1:H:228:MET:HB3	1:H:229:PRO:HD3	1.75	0.69
1:B:162:GLN:O	3:B:689:HOH:O	2.11	0.68
1:D:57:LYS:O	3:D:681:HOH:O	2.11	0.68
1:F:124:CYS:O	1:F:307:SER:OG	2.11	0.68
1:F:498:LYS:O	3:F:736:HOH:O	2.12	0.68
1:A:483:LYS:NZ	3:A:822:HOH:O	2.25	0.68
1:B:162:GLN:NE2	1:B:169:THR:OG1	2.24	0.68
1:G:483:LYS:O	3:G:784:HOH:O	2.12	0.68
1:G:279:LEU:HG	1:G:294:GLN:HG3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:MET:O	3:C:729:HOH:O	2.12	0.67
1:B:107:LYS:NZ	3:B:759:HOH:O	2.28	0.67
1:B:171:TRP:HB2	1:B:236:GLU:HG2	1.76	0.67
1:F:71:ALA:HB3	1:F:325:GLU:HG3	1.75	0.67
1:F:230:ILE:HG12	1:F:231:PRO:HD2	1.77	0.67
1:H:499:ARG:O	3:H:669:HOH:O	2.11	0.67
1:C:189:ILE:HD13	2:C:601:4VP:H5	1.77	0.66
1:G:104:LEU:HD21	1:G:340:GLU:HB2	1.78	0.66
1:H:400:HIS:HD2	1:H:459:LYS:HG2	1.60	0.66
1:F:217:GLY:HA3	1:F:265:GLU:HG2	1.77	0.66
1:E:393:THR:HG22	1:E:395:VAL:H	1.60	0.66
1:C:71:ALA:O	1:C:328:THR:HG21	1.97	0.65
1:C:394:LYS:O	3:C:788:HOH:O	2.13	0.65
1:G:347:LEU:HB3	1:G:349:ILE:HD13	1.79	0.65
1:E:373:GLN:O	3:E:803:HOH:O	2.14	0.65
1:C:228:MET:HB3	1:C:229:PRO:CD	2.26	0.64
1:A:71:ALA:HB3	1:A:325:GLU:HG3	1.79	0.64
1:G:485:TYR:HB3	1:G:489:LEU:HD23	1.80	0.64
1:F:293:SER:O	1:F:295:GLY:N	2.30	0.64
1:H:149:GLY:HA3	1:H:281:GLY:HA3	1.79	0.64
1:D:208:ASN:OD1	1:D:209:GLU:N	2.30	0.63
1:H:106:CYS:HA	1:H:109:LYS:HD2	1.80	0.63
1:E:228:MET:HG3	1:E:333:LEU:HD13	1.78	0.63
1:E:498:LYS:O	3:E:808:HOH:O	2.15	0.63
1:H:400:HIS:CD2	1:H:459:LYS:HG2	2.32	0.63
1:D:325:GLU:HA	1:D:328:THR:HG22	1.80	0.63
1:A:494:ASN:OD1	1:C:42:LYS:NZ	2.20	0.63
1:B:71:ALA:O	1:B:328:THR:HG21	1.98	0.63
1:B:325:GLU:HA	1:B:328:THR:HG22	1.81	0.62
1:A:487:LYS:NZ	3:A:842:HOH:O	2.31	0.62
1:F:415:LYS:NZ	3:F:816:HOH:O	2.31	0.62
1:H:380:GLU:O	1:H:432:MET:HE1	2.00	0.62
1:B:171:TRP:HZ3	1:B:240:VAL:HG21	1.65	0.61
1:C:277:THR:HB	1:C:297:PRO:HB2	1.82	0.61
1:G:451:ARG:HA	1:G:454:THR:HB	1.82	0.61
1:H:500:TYR:OH	3:H:644:HOH:O	2.15	0.61
1:G:373:GLN:HE21	1:G:377:THR:HG23	1.66	0.60
1:F:149:GLY:HA3	1:F:281:GLY:HA3	1.82	0.60
1:D:72:GLY:H	1:D:328:THR:HG21	1.66	0.60
1:E:149:GLY:HA3	1:E:281:GLY:HA3	1.81	0.60
1:G:135:HIS:ND1	1:G:181:ASP:OD2	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:HIS:CE1	1:F:92:PRO:HG3	2.35	0.60
1:H:449:SER:OG	1:H:450:SER:N	2.34	0.60
1:G:156:TYR:HA	1:G:173:ILE:HD11	1.83	0.60
1:G:149:GLY:HA3	1:G:281:GLY:HA3	1.84	0.59
1:H:71:ALA:O	1:H:328:THR:HG21	2.02	0.59
1:F:134:ILE:HD13	1:F:303:VAL:HG12	1.84	0.59
1:H:266:MET:HE1	1:H:314:LEU:HB2	1.84	0.59
1:A:71:ALA:O	1:A:328:THR:HG21	2.01	0.59
1:G:454:THR:HG22	1:G:456:LYS:H	1.68	0.59
1:H:210:ILE:HB	1:H:272:LEU:HB3	1.85	0.59
1:G:61:LYS:NZ	1:G:62:ASP:OD1	2.36	0.58
1:H:228:MET:HB3	1:H:229:PRO:CD	2.31	0.58
1:F:173:ILE:HG22	1:F:227:SER:HA	1.85	0.58
1:A:236:GLU:OE1	1:A:236:GLU:N	2.37	0.58
1:B:162:GLN:OE1	3:B:717:HOH:O	2.16	0.57
1:H:147:SER:OG	1:H:292:LYS:HE3	2.05	0.57
1:H:282:PRO:HG3	1:H:293:SER:H	1.68	0.57
1:E:228:MET:HE3	1:E:333:LEU:HD22	1.86	0.57
1:B:162:GLN:HE21	1:B:169:THR:HG1	1.53	0.57
1:G:18:LYS:NZ	3:G:749:HOH:O	2.37	0.57
1:D:149:GLY:HA3	1:D:281:GLY:HA3	1.87	0.57
1:E:198:ALA:HB1	1:E:274:LEU:HD11	1.87	0.57
1:E:106:CYS:HA	1:E:109:LYS:HD2	1.86	0.57
1:A:451:ARG:HD2	3:A:807:HOH:O	2.06	0.56
1:E:190:LYS:HB3	1:E:194:ILE:HD11	1.88	0.56
1:H:228:MET:HG3	1:H:330:ILE:HG23	1.86	0.56
1:H:294:GLN:H	1:H:294:GLN:CD	2.12	0.56
1:H:381:GLU:O	1:H:385:LYS:HG2	2.06	0.56
1:D:21:ASP:O	1:D:78:LYS:NZ	2.38	0.56
1:A:208:ASN:HD22	1:A:208:ASN:N	2.03	0.56
1:G:162:GLN:NE2	3:G:746:HOH:O	2.39	0.56
1:D:393:THR:HG22	1:D:395:VAL:H	1.71	0.56
1:D:106:CYS:HA	1:D:109:LYS:HD2	1.87	0.56
1:G:24[B]:ILE:CD1	1:G:49:PRO:HB2	2.34	0.55
1:G:173:ILE:HG22	1:G:227:SER:HA	1.87	0.55
1:C:86:HIS:CE1	1:C:92:PRO:HG3	2.41	0.55
1:E:104:LEU:HD11	1:E:339:LYS:HD3	1.89	0.55
1:F:173:ILE:CG2	1:F:227:SER:HA	2.37	0.55
1:D:35:GLU:HG2	1:F:489:LEU:HD11	1.87	0.55
1:F:107:LYS:HD3	1:F:340:GLU:OE1	2.05	0.55
1:G:377:THR:OG1	1:G:378:THR:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:491:ASP:OD1	3:G:765:HOH:O	2.18	0.55
1:F:12:ASP:O	1:F:16:VAL:HG23	2.07	0.55
1:G:46:SER:OG	3:G:723:HOH:O	2.18	0.54
1:F:127:HIS:NE2	1:F:310:ASP:OD1	2.39	0.54
1:G:436:ASP:HA	1:G:456:LYS:HD3	1.88	0.54
1:C:24:ILE:HD12	1:C:49:PRO:HB2	1.88	0.54
1:C:325:GLU:HA	1:C:328:THR:HG22	1.90	0.54
1:E:21:ASP:OD2	3:E:853:HOH:O	2.18	0.54
1:G:35:GLU:HG3	1:H:489:LEU:HD11	1.90	0.54
1:H:209:GLU:HA	1:H:271:THR:HG23	1.89	0.54
1:A:104:LEU:HD21	1:A:340:GLU:HB2	1.89	0.54
1:G:436:ASP:OD1	1:G:456:LYS:HD3	2.07	0.54
1:A:236:GLU:N	3:A:831:HOH:O	2.40	0.54
1:G:428:VAL:HG11	1:H:433:ALA:HB2	1.90	0.54
1:F:11:ARG:NH2	1:F:265:GLU:CD	2.66	0.53
1:F:21:ASP:O	1:F:78:LYS:NZ	2.40	0.53
1:A:149:GLY:HA3	1:A:281:GLY:HA3	1.90	0.53
1:H:451:ARG:HH21	1:H:457:GLY:HA3	1.74	0.53
1:D:387:GLY:HA3	1:D:434:PHE:CZ	2.44	0.53
1:G:72:GLY:H	1:G:328:THR:HG21	1.74	0.53
1:C:40:MET:HE1	1:C:316:VAL:HG12	1.91	0.53
1:C:21:ASP:O	1:C:78:LYS:NZ	2.41	0.52
1:A:387:GLY:HA3	1:A:434:PHE:CZ	2.44	0.52
1:B:208:ASN:HB3	1:B:273:SER:HB2	1.91	0.52
1:G:433:ALA:HB2	1:H:428:VAL:HG11	1.91	0.52
1:G:373:GLN:NE2	1:G:470:TYR:HD1	2.06	0.52
1:H:291:PHE:C	1:H:294:GLN:HE22	2.16	0.52
1:H:437:VAL:O	1:H:456:LYS:HG3	2.09	0.52
1:B:81:HIS:CD2	1:B:96:ILE:HD13	2.46	0.51
1:B:132:GLU:CD	1:B:132:GLU:H	2.18	0.51
1:F:252:LYS:HE2	1:F:256:ASN:O	2.11	0.51
1:E:162:GLN:HG2	1:E:166:LYS:HA	1.91	0.51
1:F:146:VAL:O	1:F:147:SER:HB2	2.10	0.51
1:A:160:ILE:HG22	1:A:258:LEU:HD22	1.92	0.51
1:G:24[B]:ILE:HD13	1:H:502:TYR:CZ	2.45	0.51
1:G:266:MET:HE1	1:G:314:LEU:HB2	1.91	0.51
1:F:115:ILE:HG22	1:F:247:SER:HB3	1.93	0.51
1:E:456:LYS:NZ	3:E:761:HOH:O	2.43	0.50
1:G:183:HIS:HD2	1:G:300:LEU:HG	1.76	0.50
1:B:3:LYS:HD3	1:D:234:VAL:HA	1.92	0.50
1:F:126:THR:HG22	1:F:127:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:LYS:HE2	1:G:23:LEU:HD22	1.93	0.50
1:C:209:GLU:HG3	1:C:271:THR:HG21	1.92	0.50
1:G:290:VAL:CG1	1:H:477:ILE:HB	2.38	0.50
1:A:285:GLU:OE2	2:A:601:4VP:O4'	2.30	0.50
1:F:104:LEU:HD11	1:F:340:GLU:HB2	1.94	0.50
1:C:41:ARG:NH2	1:C:324:ASP:OD2	2.44	0.49
1:D:209:GLU:HG2	1:D:271:THR:OG1	2.12	0.49
1:H:4:LEU:HD13	1:H:16:VAL:HG12	1.93	0.49
1:C:152:TYR:CZ	1:C:177:MET:HB2	2.47	0.49
1:H:24:ILE:HG12	1:H:49:PRO:HB2	1.93	0.49
1:B:106[B]:CYS:HG	1:B:239:TYR:HE1	1.58	0.49
1:F:25:GLU:HG2	1:F:52:LEU:HD23	1.95	0.49
1:G:292:LYS:O	1:G:293:SER:HB2	2.13	0.49
1:G:375:LEU:HB3	1:G:377:THR:HG22	1.94	0.49
1:A:290:VAL:HB	1:C:477:ILE:HB	1.93	0.49
1:C:266:MET:HE1	1:C:314:LEU:HB2	1.95	0.49
1:F:112:LEU:O	3:F:770:HOH:O	2.19	0.49
1:C:133:LYS:NZ	3:C:802:HOH:O	2.46	0.49
1:H:435:ASP:HA	1:H:457:GLY:CA	2.42	0.49
1:B:478:THR:HG21	1:B:483:LYS:HE3	1.94	0.49
1:E:436:ASP:OD1	1:E:436:ASP:N	2.46	0.49
1:D:152:TYR:CZ	1:D:177:MET:HB2	2.48	0.49
1:G:379:PRO:HD3	1:G:470:TYR:CD1	2.48	0.49
1:H:387:GLY:HA3	1:H:434:PHE:CZ	2.48	0.49
1:D:272:LEU:HD11	1:D:299:PRO:HB2	1.94	0.48
1:C:228:MET:SD	2:C:601:4VP:H3	2.52	0.48
1:C:121:SER:O	1:C:123:PRO:HD3	2.14	0.48
1:H:4:LEU:N	3:H:680:HOH:O	2.45	0.48
1:A:278:HIS:HB2	1:A:300:LEU:HD13	1.95	0.48
1:G:280:GLU:N	1:G:294:GLN:OE1	2.47	0.48
1:B:489:LEU:HD11	1:E:35:GLU:HG2	1.94	0.48
1:F:11:ARG:NH2	1:F:265:GLU:OE1	2.47	0.48
1:D:477:ILE:HB	1:F:290:VAL:HB	1.96	0.48
1:F:160:ILE:HB	1:F:213:ALA:HB3	1.95	0.48
1:F:106:CYS:HA	1:F:109:LYS:HD2	1.95	0.47
1:B:149:GLY:HA3	1:B:281:GLY:HA3	1.95	0.47
1:E:111:PRO:HB2	1:E:238:ASP:HB3	1.95	0.47
1:C:230:ILE:HG22	3:C:811:HOH:O	2.13	0.47
1:B:21:ASP:O	1:B:78:LYS:NZ	2.48	0.47
1:F:379:PRO:HG3	1:F:470:TYR:CE1	2.49	0.47
1:A:210:ILE:HB	1:A:272:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:HIS:CG	1:A:297:PRO:HD2	2.50	0.47
1:D:436:ASP:OD1	1:D:436:ASP:N	2.47	0.47
1:F:18:LYS:HG2	1:F:23:LEU:HD22	1.96	0.47
1:G:373:GLN:NE2	1:G:377:THR:HG23	2.28	0.47
1:G:465:ILE:HB	1:G:470:TYR:CE2	2.50	0.47
1:H:173:ILE:HG21	1:H:227:SER:HA	1.97	0.47
1:A:239:TYR:OH	3:A:791:HOH:O	2.20	0.47
1:C:107:LYS:HE3	1:C:340:GLU:OE1	2.14	0.47
1:D:57:LYS:NZ	3:D:678:HOH:O	2.47	0.47
1:G:366:LYS:HE3	1:G:407:ASP:HA	1.96	0.47
1:D:266:MET:HE1	1:D:314:LEU:HB2	1.97	0.47
1:B:9:GLU:HB2	1:B:12:ASP:HB2	1.96	0.46
1:E:293:SER:C	3:E:855:HOH:O	2.58	0.46
1:A:325:GLU:HA	1:A:328:THR:HG22	1.97	0.46
1:G:373:GLN:HG2	1:G:376:LYS:HA	1.97	0.46
1:H:393:THR:HG22	1:H:395:VAL:H	1.79	0.46
1:B:208:ASN:N	3:B:763:HOH:O	2.47	0.46
1:E:448:GLN:OE1	3:E:708:HOH:O	2.21	0.46
1:E:132:GLU:HG2	1:E:133:LYS:HG2	1.97	0.46
1:G:477:ILE:HB	1:H:290:VAL:CG1	2.44	0.46
3:D:619:HOH:O	1:F:451:ARG:HD2	2.15	0.46
1:F:56:LEU:HD11	1:F:66:ILE:HG13	1.97	0.46
1:C:164:PRO:CD	1:C:200:SER:HB3	2.45	0.46
1:B:162:GLN:N	3:B:689:HOH:O	2.34	0.46
1:D:322:CYS:HA	1:D:323:THR:HA	1.76	0.46
1:G:162:GLN:OE1	1:G:166:LYS:HG3	2.16	0.46
1:F:86:HIS:HE1	1:F:92:PRO:HG3	1.81	0.46
1:G:361:LEU:HD12	1:H:422:VAL:HG12	1.98	0.46
1:H:377:THR:OG1	1:H:378:THR:N	2.49	0.46
1:C:190:LYS:NZ	1:C:196:GLN:OE1	2.28	0.45
1:H:355:PRO:CD	1:H:364:ILE:HD13	2.46	0.45
1:C:224:LEU:O	1:C:227:SER:HB2	2.16	0.45
1:D:40:MET:HE3	1:D:69:CYS:H	1.81	0.45
1:G:173:ILE:HD12	1:G:223:ILE:HD11	1.99	0.45
1:H:86:HIS:CE1	1:H:92:PRO:HG3	2.50	0.45
1:B:377:THR:OG1	1:B:378:THR:N	2.48	0.45
1:D:41:ARG:HD3	1:D:45:GLU:OE2	2.16	0.45
1:D:228:MET:HA	1:D:228:MET:HE2	1.99	0.45
1:E:452:SER:HA	1:E:455:MET:HE2	1.97	0.45
1:H:378:THR:OG1	3:H:726:HOH:O	2.20	0.45
1:B:209:GLU:HA	1:B:271:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:TRP:HB2	1:D:236:GLU:CG	2.46	0.45
1:F:387:GLY:HA3	1:F:434:PHE:CZ	2.52	0.45
1:G:380:GLU:OE1	1:G:380:GLU:N	2.45	0.45
1:G:401:GLU:HG3	1:G:460:CYS:SG	2.56	0.45
1:F:41:ARG:NH2	1:F:324:ASP:OD2	2.49	0.45
1:A:24:ILE:HG12	1:A:49:PRO:HB2	1.99	0.45
1:G:372:LEU:O	1:G:375:LEU:HB2	2.17	0.45
1:A:450:SER:O	1:A:453:LYS:HG3	2.16	0.45
1:D:18:LYS:HG3	1:D:23:LEU:HD22	1.98	0.45
1:E:322:CYS:HA	1:E:323:THR:HA	1.82	0.44
1:G:293:SER:OG	1:G:294:GLN:N	2.49	0.44
1:H:21:ASP:O	1:H:78:LYS:NZ	2.49	0.44
1:A:354:MET:HE2	1:A:354:MET:HB3	1.87	0.44
1:D:256:ASN:HB2	3:D:785:HOH:O	2.17	0.44
1:E:466:PHE:HB2	1:E:469:GLN:HG3	2.00	0.44
1:F:272:LEU:HD11	1:F:299:PRO:HB3	2.00	0.44
1:G:18:LYS:HG3	1:G:23:LEU:HD22	1.98	0.44
1:A:42:LYS:HD2	1:C:481:PHE:CE2	2.52	0.44
1:B:26:ILE:HA	3:B:661:HOH:O	2.16	0.44
1:B:451:ARG:HD2	3:B:622:HOH:O	2.18	0.44
1:E:40:MET:HE1	1:E:316:VAL:HG12	1.99	0.44
1:F:6:PRO:O	1:F:220:PRO:HG2	2.17	0.44
1:G:468:GLN:CD	1:G:474:PHE:HD1	2.26	0.44
1:E:187:LEU:HD21	1:E:189:ILE:HD11	2.00	0.44
1:F:438:THR:O	1:F:459:LYS:HE3	2.18	0.44
1:B:41:ARG:HD3	1:B:44:TYR:HD2	1.83	0.44
1:E:104:LEU:HD22	1:E:340:GLU:OE2	2.17	0.44
1:E:223:ILE:HD12	1:E:223:ILE:HA	1.92	0.44
1:F:294:GLN:H	1:F:294:GLN:HG2	1.54	0.44
1:F:442:LEU:HD12	1:F:442:LEU:HA	1.88	0.44
1:H:57:LYS:NZ	3:H:711:HOH:O	2.50	0.44
1:H:326:THR:O	1:H:330:ILE:HB	2.18	0.44
1:A:208:ASN:N	1:A:208:ASN:ND2	2.66	0.44
1:B:74:ARG:NH2	1:B:78:LYS:O	2.44	0.44
1:G:91:ASP:HA	1:G:92:PRO:HD2	1.86	0.44
1:A:489:LEU:HD11	1:C:35:GLU:HG3	1.99	0.43
1:C:438:THR:O	1:C:459:LYS:HE3	2.17	0.43
1:F:104:LEU:HA	1:F:104:LEU:HD12	1.74	0.43
1:G:373:GLN:HG2	1:G:376:LYS:CA	2.48	0.43
1:B:452:SER:O	1:B:455:MET:HE2	2.18	0.43
1:C:230:ILE:HD11	1:C:239:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LYS:HD2	1:E:196:GLN:OE1	2.18	0.43
1:F:164:PRO:HG3	1:F:201:TRP:CD2	2.53	0.43
1:C:18:LYS:HE2	1:C:23:LEU:HD22	2.00	0.43
1:E:451:ARG:HD2	3:E:732:HOH:O	2.17	0.43
1:H:104:LEU:HD21	1:H:340:GLU:HB2	2.01	0.43
1:H:322:CYS:HA	1:H:323:THR:HA	1.73	0.43
1:A:452:SER:O	1:A:455:MET:HE2	2.17	0.43
1:B:322:CYS:HA	1:B:323:THR:HA	1.80	0.43
1:H:91:ASP:HA	1:H:92:PRO:HD3	1.87	0.43
1:H:435:ASP:HA	1:H:457:GLY:HA2	2.00	0.43
1:B:228:MET:HB2	1:B:333:LEU:HD12	2.00	0.43
1:E:173:ILE:HG22	1:E:226:SER:O	2.19	0.43
1:H:48:LEU:HB3	1:H:49:PRO:HD2	2.01	0.43
1:A:175:ARG:CZ	1:A:187:LEU:HD22	2.49	0.43
1:C:422:VAL:HG12	1:C:423:THR:HG23	2.00	0.43
1:C:471:GLU:OE1	1:C:472:ARG:NH1	2.51	0.43
1:F:306:MET:HE2	1:F:306:MET:HB3	1.80	0.43
1:H:133:LYS:CE	3:H:690:HOH:O	2.65	0.43
1:H:167:LYS:HD3	1:H:167:LYS:HA	1.49	0.43
1:A:107:LYS:NZ	3:A:791:HOH:O	2.52	0.43
1:H:384:LYS:HE3	1:H:392:ARG:NH2	2.33	0.43
1:A:158:MET:HE3	1:A:160:ILE:HD11	2.01	0.42
1:C:415:LYS:HG2	3:C:799:HOH:O	2.19	0.42
1:E:208:ASN:HA	1:E:273:SER:HA	2.00	0.42
1:E:220:PRO:O	1:E:223:ILE:HG22	2.19	0.42
1:G:173:ILE:CG2	1:G:227:SER:HA	2.48	0.42
1:H:31:ASP:O	1:H:35:GLU:HB2	2.19	0.42
3:A:721:HOH:O	1:C:451:ARG:HD2	2.18	0.42
1:F:132:GLU:OE2	1:F:182:LYS:NZ	2.49	0.42
1:C:333:LEU:O	1:C:337:GLU:HG2	2.20	0.42
1:H:228:MET:HG2	1:H:330:ILE:HG12	2.02	0.42
1:H:432:MET:HE3	1:H:432:MET:HB2	1.79	0.42
1:E:387:GLY:HA3	1:E:434:PHE:CZ	2.55	0.42
1:G:187:LEU:HA	1:G:298:CYS:SG	2.60	0.42
1:A:10:PHE:O	1:A:13:PHE:HB3	2.20	0.42
1:B:10:PHE:O	1:B:13:PHE:HB3	2.20	0.42
1:B:270:GLY:HA3	1:B:302:THR:O	2.20	0.42
1:F:223:ILE:HD12	1:F:223:ILE:HA	1.94	0.42
1:H:104:LEU:HD23	1:H:104:LEU:HA	1.78	0.42
1:H:384:LYS:HD2	1:H:434:PHE:CZ	2.54	0.42
1:G:325:GLU:HA	1:G:328:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:469:GLN:HG2	3:H:606:HOH:O	2.20	0.42
1:G:25:GLU:OE2	1:G:54:LYS:NZ	2.53	0.42
1:B:438:THR:O	1:B:459:LYS:HE3	2.20	0.42
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.83	0.42
1:B:272:LEU:HD12	1:B:273:SER:N	2.34	0.42
1:C:228:MET:HG2	1:C:330:ILE:HD13	2.01	0.42
1:C:387:GLY:HA3	1:C:434:PHE:CZ	2.55	0.42
1:E:227:SER:HB2	1:E:333:LEU:CD1	2.49	0.42
1:E:284:GLY:CA	1:E:290:VAL:HG22	2.49	0.42
2:A:601:4VP:H1	2:A:601:4VP:H4	1.81	0.41
1:D:46:SER:HB2	1:D:48:LEU:HG	2.02	0.41
1:E:54:LYS:NZ	3:E:859:HOH:O	2.47	0.41
1:E:293:SER:HB2	3:E:831:HOH:O	2.20	0.41
1:F:252:LYS:NZ	3:F:803:HOH:O	2.23	0.41
1:H:17:LEU:HD12	1:H:17:LEU:HA	1.86	0.41
1:H:132:GLU:OE2	1:H:133:LYS:HE2	2.20	0.41
1:C:322:CYS:HA	1:C:323:THR:HA	1.70	0.41
1:C:418:ILE:HD12	1:C:418:ILE:HA	1.90	0.41
1:F:180:ASP:CG	1:F:183:HIS:HD1	2.28	0.41
1:F:231:PRO:O	1:F:234:VAL:HG12	2.20	0.41
1:H:86:HIS:HE1	1:H:92:PRO:HG3	1.85	0.41
1:B:266:MET:HE1	1:B:314:LEU:HB2	2.02	0.41
1:C:277:THR:CB	1:C:297:PRO:HB2	2.48	0.41
1:D:302:THR:OG1	3:D:676:HOH:O	2.21	0.41
1:E:204:ILE:HG13	1:E:206:LYS:HG2	2.02	0.41
1:G:322:CYS:HA	1:G:323:THR:HA	1.73	0.41
1:B:42:LYS:HE3	1:E:494:ASN:OD1	2.21	0.41
1:B:63:LEU:HA	1:B:64:PHE:HB3	2.02	0.41
1:C:161:LEU:HB3	1:C:197:ILE:HG21	2.02	0.41
1:C:104:LEU:HD21	1:C:340:GLU:HB2	2.02	0.41
1:C:278:HIS:HB2	1:C:300:LEU:HD13	2.02	0.41
1:D:497:TRP:CZ3	1:F:42:LYS:HD3	2.56	0.41
1:A:322:CYS:HA	1:A:323:THR:HA	1.79	0.41
1:G:63:LEU:HD21	1:G:308:TYR:CG	2.55	0.41
1:H:230:ILE:HG21	1:H:236:GLU:OE2	2.21	0.41
1:C:210:ILE:HB	1:C:272:LEU:HG	2.03	0.41
1:C:442:LEU:HD23	1:C:442:LEU:HA	1.66	0.41
1:G:400:HIS:ND1	1:G:459:LYS:HG2	2.36	0.41
1:G:467:ARG:H	1:H:448:GLN:HE22	1.69	0.41
1:B:440:PHE:HA	1:B:441:PRO:HD3	1.94	0.41
1:D:129:LEU:HD22	1:D:133:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:LEU:HD22	1:E:340:GLU:CD	2.46	0.41
1:G:369:LEU:HD23	1:G:369:LEU:HA	1.87	0.41
1:A:42:LYS:HE3	1:C:494:ASN:OD1	2.21	0.40
1:C:6:PRO:HG3	1:C:16:VAL:HG11	2.02	0.40
1:D:162:GLN:N	3:D:677:HOH:O	2.34	0.40
1:E:380:GLU:O	1:E:432:MET:HE1	2.21	0.40
1:G:103:LEU:HD23	1:G:103:LEU:HA	1.91	0.40
1:H:342:ALA:HB2	1:H:390:TYR:OH	2.21	0.40
1:C:164:PRO:HD2	1:C:200:SER:HB3	2.03	0.40
1:C:404:LEU:O	1:C:464:CYS:HB2	2.22	0.40
1:F:40:MET:HE3	1:F:69:CYS:H	1.86	0.40
1:F:94:THR:HG22	1:F:98:GLU:HB2	2.03	0.40
1:G:46:SER:HB2	1:G:48:LEU:HG	2.02	0.40
1:A:487:LYS:HA	1:A:490:VAL:HB	2.02	0.40
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.80	0.40
1:H:434:PHE:O	1:H:457:GLY:HA2	2.21	0.40
1:A:152:TYR:CZ	1:A:177:MET:HB2	2.56	0.40
1:A:266:MET:HE1	1:A:314:LEU:HB2	2.03	0.40
1:E:401:GLU:HG3	1:E:460:CYS:SG	2.62	0.40
1:H:236:GLU:O	1:H:240:VAL:HG23	2.21	0.40
1:H:472:ARG:CZ	1:H:472:ARG:HB2	2.52	0.40
1:B:208:ASN:OD1	1:B:275:THR:HG23	2.21	0.40
1:B:393:THR:CG2	1:B:395:VAL:H	2.31	0.40
1:F:75:SER:HB2	1:F:77:GLU:OE2	2.21	0.40
1:F:126:THR:HG22	1:F:127:HIS:HD2	1.87	0.40
1:G:373:GLN:CG	1:G:377:THR:H	2.34	0.40
1:H:210:ILE:HA	1:H:211:PRO:HD3	1.94	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:C:167:LYS:NZ	1:G:98:GLU:OE2[2_756]	2.15	0.05

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	464/503 (92%)	448 (97%)	15 (3%)	1 (0%)	43	50
1	B	470/503 (93%)	453 (96%)	17 (4%)	0	100	100
1	C	499/503 (99%)	476 (95%)	21 (4%)	2 (0%)	30	32
1	D	475/503 (94%)	455 (96%)	19 (4%)	1 (0%)	43	50
1	E	486/503 (97%)	472 (97%)	14 (3%)	0	100	100
1	F	499/503 (99%)	482 (97%)	16 (3%)	1 (0%)	43	50
1	G	465/503 (92%)	445 (96%)	18 (4%)	2 (0%)	30	32
1	H	478/503 (95%)	453 (95%)	23 (5%)	2 (0%)	30	32
All	All	3836/4024 (95%)	3684 (96%)	143 (4%)	9 (0%)	43	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	228	MET
1	F	294	GLN
1	G	436	ASP
1	H	228	MET
1	C	293	SER
1	D	230	ILE
1	G	428	VAL
1	H	233	GLY
1	A	119	VAL

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	413/438 (94%)	404 (98%)	9 (2%)	45	58
1	B	420/438 (96%)	408 (97%)	12 (3%)	37	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	436/438 (100%)	416 (95%)	20 (5%)	24	31
1	D	422/438 (96%)	404 (96%)	18 (4%)	26	33
1	E	429/438 (98%)	421 (98%)	8 (2%)	50	63
1	F	436/438 (100%)	419 (96%)	17 (4%)	28	37
1	G	415/438 (95%)	398 (96%)	17 (4%)	27	35
1	H	421/438 (96%)	404 (96%)	17 (4%)	28	36
All	All	3392/3504 (97%)	3274 (96%)	118 (4%)	32	41

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	61	LYS
1	A	172	SER
1	A	208	ASN
1	A	226	SER
1	A	271	THR
1	A	276	ASP
1	A	328	THR
1	A	460	CYS
1	B	41	ARG
1	B	132	GLU
1	B	167	LYS
1	B	172	SER
1	B	246	GLU
1	B	271	THR
1	B	290	VAL
1	B	307	SER
1	B	328	THR
1	B	333	LEU
1	B	393	THR
1	B	460	CYS
1	C	24	ILE
1	C	77	GLU
1	C	107	LYS
1	C	132	GLU
1	C	161	LEU
1	C	166	LYS
1	C	204	ILE
1	C	209	GLU

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Mol	Chain	Res	Type
1	C	227	SER
1	C	228	MET
1	C	230	ILE
1	C	236	GLU
1	C	271	THR
1	C	272	LEU
1	C	275	THR
1	C	345	SER
1	C	384	LYS
1	C	422	VAL
1	C	460	CYS
1	C	483	LYS
1	D	41	ARG
1	D	115	ILE
1	D	172	SER
1	D	188	VAL
1	D	209	GLU
1	D	230	ILE
1	D	232	GLU
1	D	234	VAL
1	D	246	GLU
1	D	251	VAL
1	D	271	THR
1	D	274	LEU
1	D	275	THR
1	D	344	GLU
1	D	385	LYS
1	D	393	THR
1	D	460	CYS
1	D	483	LYS
1	E	17	LEU
1	E	23	LEU
1	E	133	LYS
1	E	187	LEU
1	E	275	THR
1	E	467	ARG
1	E	483	LYS
1	E	495	GLU
1	F	3	LYS
1	F	11	ARG
1	F	41	ARG
1	F	77	GLU

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Mol	Chain	Res	Type
1	F	104	LEU
1	F	121	SER
1	F	187	LEU
1	F	197	ILE
1	F	200	SER
1	F	247	SER
1	F	254	GLU
1	F	271	THR
1	F	272	LEU
1	F	393	THR
1	F	394	LYS
1	F	460	CYS
1	F	483	LYS
1	G	24[A]	ILE
1	G	24[B]	ILE
1	G	134	ILE
1	G	182	LYS
1	G	187	LEU
1	G	220	PRO
1	G	272	LEU
1	G	279	LEU
1	G	290	VAL
1	G	294	GLN
1	G	298	CYS
1	G	328	THR
1	G	373	GLN
1	G	377	THR
1	G	425	HIS
1	G	460	CYS
1	G	472	ARG
1	H	17	LEU
1	H	56	LEU
1	H	167	LYS
1	H	172	SER
1	H	251	VAL
1	H	271	THR
1	H	290	VAL
1	H	328	THR
1	H	333	LEU
1	H	381	GLU
1	H	394	LYS
1	H	400	HIS

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Mol	Chain	Res	Type
1	H	435	ASP
1	H	448	GLN
1	H	450	SER
1	H	452	SER
1	H	454	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	33	ASN
1	A	135	HIS
1	A	278	HIS
1	B	162	GLN
1	B	183	HIS
1	B	469	GLN
1	C	33	ASN
1	C	193	HIS
1	C	208	ASN
1	D	33	ASN
1	E	162	GLN
1	E	170	ASN
1	F	294	GLN
1	F	468	GLN
1	G	170	ASN
1	G	183	HIS
1	H	208	ASN
1	H	311	ASN
1	H	400	HIS
1	H	448	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
2	4VP	E	601	-	9,9,9	0.83	0	11,11,11	0.77	0
2	4VP	G	601	-	9,9,9	0.77	0	11,11,11	0.78	0
2	4VP	F	601	-	9,9,9	0.82	0	11,11,11	0.68	0
2	4VP	A	601	-	9,9,9	0.68	0	11,11,11	0.95	0
2	4VP	C	601	-	9,9,9	0.69	0	11,11,11	0.86	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	4VP	E	601	-	-	2/2/2/2	0/1/1/1
2	4VP	G	601	-	-	0/2/2/2	0/1/1/1
2	4VP	F	601	-	-	2/2/2/2	0/1/1/1
2	4VP	A	601	-	-	0/2/2/2	0/1/1/1
2	4VP	C	601	-	-	0/2/2/2	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	4VP	C2'-C1'-C3-C2

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Mol	Chain	Res	Type	Atoms
2	F	601	4VP	C6'-C1'-C3-C2
2	E	601	4VP	C6'-C1'-C3-C2
2	E	601	4VP	C2'-C1'-C3-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	4VP	1	0
2	A	601	4VP	2	0
2	C	601	4VP	2	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	472/503 (93%)	-0.09	7 (1%) 72 76	22, 37, 66, 87	0
1	B	476/503 (94%)	-0.11	7 (1%) 72 76	23, 36, 66, 110	2 (0%)
1	C	501/503 (99%)	-0.05	5 (0%) 79 82	25, 40, 64, 87	0
1	D	480/503 (95%)	-0.13	12 (2%) 58 64	19, 35, 66, 95	1 (0%)
1	E	492/503 (97%)	-0.11	3 (0%) 85 88	24, 37, 62, 82	0
1	F	501/503 (99%)	0.14	10 (1%) 65 70	22, 46, 75, 94	0
1	G	472/503 (93%)	0.39	20 (4%) 40 46	24, 53, 85, 110	1 (0%)
1	H	481/503 (95%)	0.33	26 (5%) 31 37	26, 46, 84, 107	1 (0%)
All	All	3875/4024 (96%)	0.04	90 (2%) 61 66	19, 40, 74, 110	5 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	168	TRP	5.1
1	B	168	TRP	5.1
1	D	296	HIS	5.0
1	H	207	ALA	4.3
1	F	281	GLY	4.3
1	H	448	GLN	3.9
1	B	281	GLY	3.9
1	G	168	TRP	3.9
1	F	293	SER	3.8
1	B	171	TRP	3.7
1	H	291	PHE	3.6
1	F	209	GLU	3.5
1	G	476	TYR	3.5
1	H	281	GLY	3.4
1	A	295	GLY	3.4
1	D	281	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	295	GLY	3.3
1	E	281	GLY	3.3
1	H	230	ILE	3.3
1	A	296	HIS	3.2
1	H	388	ASP	3.2
1	C	281	GLY	3.1
1	G	473	SER	3.1
1	F	296	HIS	3.0
1	G	281	GLY	3.0
1	H	296	HIS	3.0
1	F	294	GLN	3.0
1	H	454	THR	2.9
1	A	69	CYS	2.9
1	H	381	GLU	2.9
1	G	475	ASP	2.9
1	D	171	TRP	2.9
1	H	231	PRO	2.8
1	G	474	PHE	2.8
1	F	208	ASN	2.8
1	H	450	SER	2.8
1	C	296	HIS	2.8
1	D	168	TRP	2.8
1	D	230	ILE	2.8
1	A	293	SER	2.8
1	H	293	SER	2.8
1	F	295	GLY	2.7
1	B	187	LEU	2.7
1	H	187	LEU	2.7
1	H	232	GLU	2.7
1	G	72	GLY	2.6
1	H	233	GLY	2.6
1	D	188	VAL	2.6
1	E	194	ILE	2.6
1	A	281	GLY	2.5
1	D	293	SER	2.5
1	G	374	ALA	2.5
1	G	488	GLY	2.5
1	G	235	SER	2.4
1	H	234	VAL	2.4
1	G	187	LEU	2.4
1	H	295	GLY	2.4
1	H	384	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	171	TRP	2.4
1	G	436	ASP	2.4
1	H	438	THR	2.3
1	E	228	MET	2.3
1	G	435	ASP	2.3
1	G	164	PRO	2.3
1	G	372	LEU	2.3
1	C	168	TRP	2.2
1	F	168	TRP	2.2
1	A	208	ASN	2.2
1	G	393	THR	2.2
1	H	473	SER	2.2
1	G	373	GLN	2.2
1	G	454	THR	2.2
1	H	449	SER	2.2
1	B	170	ASN	2.1
1	G	209	GLU	2.1
1	D	464	CYS	2.1
1	D	239	TYR	2.1
1	C	3	LYS	2.1
1	G	208	ASN	2.1
1	H	229	PRO	2.1
1	D	232	GLU	2.1
1	B	297	PRO	2.1
1	F	253	CYS	2.1
1	D	238	ASP	2.1
1	H	453	LYS	2.0
1	A	322	CYS	2.0
1	F	254	GLU	2.0
1	H	170	ASN	2.0
1	D	229	PRO	2.0
1	B	167	LYS	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

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	4VP	E	601	9/9	0.79	0.14	40,41,62,68	0
2	4VP	A	601	9/9	0.82	0.17	55,58,64,66	0
2	4VP	G	601	9/9	0.82	0.14	49,51,61,66	0
2	4VP	F	601	9/9	0.86	0.13	42,45,53,57	0
2	4VP	C	601	9/9	0.86	0.12	48,50,54,58	0

6.5 Other polymers

There are no such residues in this entry.