



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:50 PM UTC

PDB ID : 1SME / pdb_00001sme
Title : PLASMEPSIN II, A HEMOGLOBIN-DEGRADING ENZYME FROM PLASMODIUM FALCIPARUM, IN COMPLEX WITH PEPSTATIN A
Authors : Silva, A.M.; Lee, A.Y.; Gulnik, S.V.; Goldberg, D.E.; Erickson, J.W.
Deposited on : 1996-06-11
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

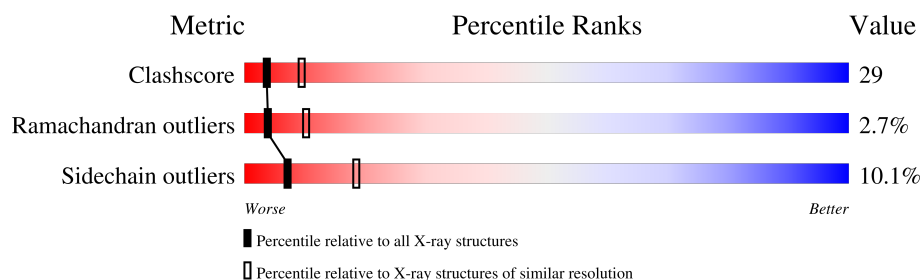
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	329	49% 42% 8% .
1	B	329	41% 47% 10% .
2	C	6	17% 33% 33% 17%
2	D	6	17% 33% 33% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6723 atoms, of which 1298 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 PLASMEPSIN II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	H	N	O	S	0	0	0
			3134	1689	527	404	503	11			
1	B	329	Total	C	H	N	O	S	0	0	0
			3134	1689	527	404	503	11			

- Molecule 2 is a protein called Pepstatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	H	N	O	0	0	0
			55	34	7	5	9			
2	D	6	Total	C	H	N	O	0	0	0
			55	34	7	5	9			

- Molecule 3 is water.

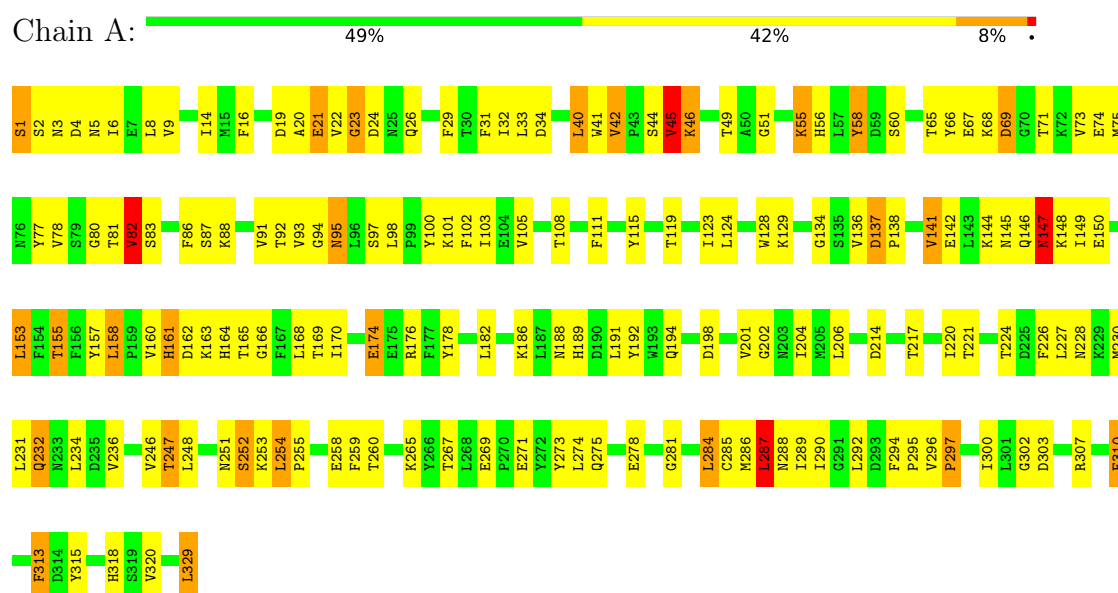
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	77	Total	H	O	0	0
			231	154	77		
3	B	34	Total	H	O	0	0
			102	68	34		
3	C	1	Total	H	O	0	0
			3	2	1		
3	D	3	Total	H	O	0	0
			9	6	3		

3 Residue-property plots

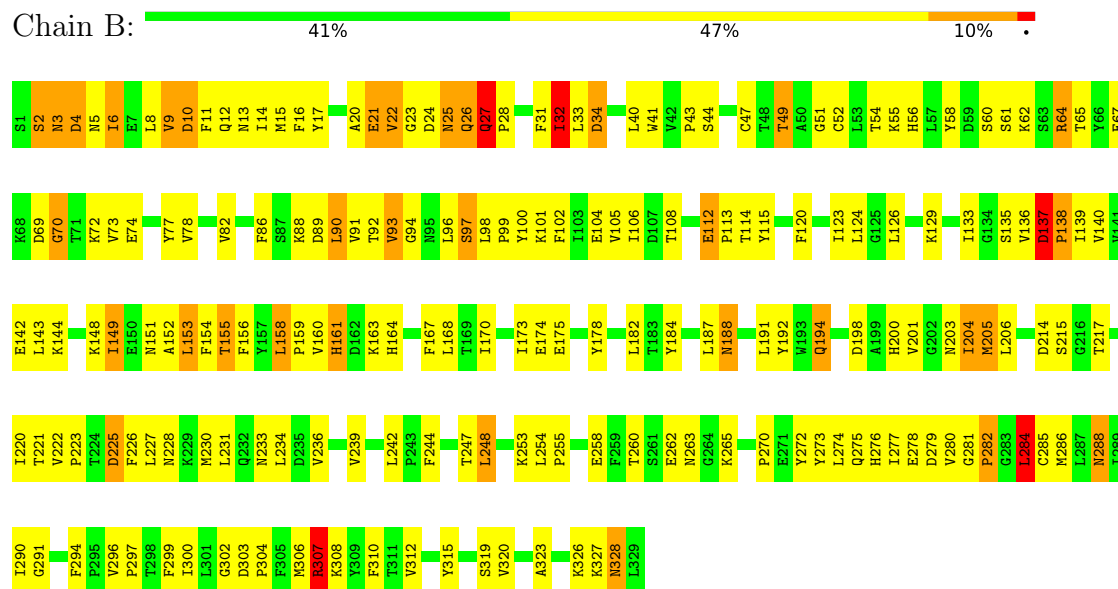
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: PLASMEPSIN II



• Molecule 1: PLASMEPSIN II



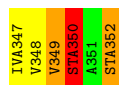
● Molecule 2: Pepstatin

Chain C:  17% 33% 33% 17%



● Molecule 2: Pepstatin

Chain D:  17% 33% 33% 17%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.10 Å 142.10 Å 97.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	74.3 (8.00-2.70)	Depositor
R_{merge}	0.94	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6723	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.68	0/2674	1.26	34/3638 (0.9%)
1	B	0.67	1/2674 (0.0%)	1.21	27/3638 (0.7%)
2	C	0.59	0/17	2.38	1/21 (4.8%)
2	D	0.63	0/17	1.38	0/21
All	All	0.67	1/5382 (0.0%)	1.24	62/7318 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	D	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ARG	CZ-NH2	6.20	1.41	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ILE	N-CA-C	-10.16	93.07	107.80
1	A	248	LEU	N-CA-C	-10.01	93.84	109.76
1	A	40	LEU	CD1-CG-CD2	-9.17	90.63	110.80
1	A	287	LEU	N-CA-C	8.99	122.05	111.71
1	B	8	LEU	CD1-CG-CD2	-8.46	92.20	110.80
1	A	23	GLY	N-CA-C	-8.24	102.51	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LEU	CD1-CG-CD2	-8.07	93.04	110.80
1	B	3	ASN	N-CA-C	7.90	121.27	108.63
1	A	178	TYR	N-CA-C	7.82	122.22	109.72
1	B	137	ASP	CA-C-N	7.58	129.31	119.84
1	B	137	ASP	C-N-CA	7.58	129.31	119.84
1	B	248	LEU	N-CA-C	-7.46	98.76	109.96
2	C	348	VAL	CG1-CB-CG2	-7.31	94.71	110.80
1	B	32	ILE	N-CA-C	-7.30	96.49	106.85
1	B	192	TYR	N-CA-C	-7.26	99.71	110.46
1	B	82	VAL	CG1-CB-CG2	-7.09	95.19	110.80
1	A	9	VAL	CG1-CB-CG2	-7.08	95.21	110.80
1	B	27	GLN	CA-C-N	7.02	126.78	119.76
1	B	27	GLN	C-N-CA	7.02	126.78	119.76
1	B	153	LEU	CD1-CG-CD2	-7.00	95.41	110.80
1	A	202	GLY	N-CA-C	-6.92	96.79	113.18
1	B	133	ILE	N-CA-C	-6.85	100.74	109.58
1	B	239	VAL	N-CA-C	-6.69	102.88	108.63
1	A	56	HIS	N-CA-C	-6.43	98.78	109.46
1	A	192	TYR	N-CA-C	-6.35	100.58	110.17
1	B	188	ASN	N-CA-C	-6.35	102.90	112.04
1	B	263	ASN	N-CA-C	6.21	120.59	112.89
1	A	296	VAL	CA-C-N	6.18	127.57	119.84
1	A	296	VAL	C-N-CA	6.18	127.57	119.84
1	B	112	GLU	N-CA-C	-6.14	102.12	110.36
1	A	42	VAL	CG1-CB-CG2	6.06	124.13	110.80
1	B	10	ASP	N-CA-C	6.03	118.35	108.52
1	A	34	ASP	N-CA-C	5.97	118.85	107.75
1	A	246	VAL	N-CA-C	5.96	117.16	108.58
1	A	329	LEU	CD1-CG-CD2	5.73	123.41	110.80
1	B	34	ASP	N-CA-C	5.73	118.02	109.25
1	B	262	GLU	N-CA-C	-5.72	105.05	111.28
1	B	9	VAL	CG1-CB-CG2	5.69	123.32	110.80
1	A	254	LEU	CA-C-N	5.65	125.63	120.21
1	A	254	LEU	C-N-CA	5.65	125.63	120.21
1	A	55	LYS	N-CA-C	5.60	118.11	110.55
1	B	284	LEU	N-CA-C	5.57	119.18	110.32
1	A	204	ILE	CB-CA-C	-5.54	104.26	110.96
1	A	182	LEU	N-CA-C	-5.51	101.57	110.32
1	A	232	GLN	N-CA-C	5.50	118.10	111.40
1	A	82	VAL	CG1-CB-CG2	5.48	122.85	110.80
1	A	2	SER	N-CA-C	-5.45	105.30	112.72
1	B	204	ILE	CB-CA-C	-5.43	105.43	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	TYR	N-CA-C	5.42	118.07	109.24
1	B	320	VAL	N-CA-C	-5.38	99.76	107.78
1	A	33	LEU	CD1-CG-CD2	5.35	122.58	110.80
1	B	320	VAL	CG1-CB-CG2	-5.33	99.07	110.80
1	A	320	VAL	N-CA-C	-5.31	100.82	108.89
1	A	45	VAL	CG1-CB-CG2	-5.30	99.14	110.80
1	B	158	LEU	N-CA-C	5.27	117.16	109.84
1	A	310	PHE	N-CA-C	-5.23	102.12	109.96
1	B	328	ASN	N-CA-C	5.21	116.58	109.18
1	A	134	GLY	N-CA-C	-5.12	108.21	115.43
1	A	224	THR	N-CA-C	5.08	119.75	111.37
1	B	22	VAL	CG1-CB-CG2	-5.06	99.66	110.80
1	A	19	ASP	N-CA-C	5.05	117.92	110.59
1	A	220	ILE	N-CA-C	-5.05	99.99	107.51

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	350	STA	Mainchain,Peptide
2	D	349	VAL	Peptide
2	D	350	STA	Mainchain,Peptide

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	2607	527	2536	122	0
1	B	2607	527	2536	180	0
2	C	48	7	61	5	0
2	D	48	7	60	10	0
3	A	77	154	0	0	0
3	B	34	68	0	0	0
3	C	1	2	0	0	0
3	D	3	6	0	0	0
All	All	5425	1298	5193	305	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 29.

All (305) 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:B:276:HIS:HA	1:B:285:CYS:HB3	1.34	1.05
1:B:221:THR:HB	1:B:300:ILE:HB	1.42	0.97
1:B:44:SER:HB2	1:B:104:GLU:HG2	1.53	0.90
1:B:234:LEU:HD11	1:B:254:LEU:HD23	1.51	0.90
1:A:6:ILE:HD11	1:A:93:VAL:HG12	1.55	0.88
1:B:20:ALA:HB3	1:B:31:PHE:CE2	2.09	0.85
1:B:49:THR:HG22	1:B:52:CYS:H	1.41	0.84
1:B:276:HIS:HA	1:B:285:CYS:CB	2.10	0.82
1:A:221:THR:HB	1:A:300:ILE:HB	1.61	0.80
1:B:98:LEU:HD22	1:B:143:LEU:HD21	1.63	0.80
1:B:160:VAL:HG11	1:B:163:LYS:HD3	1.63	0.80
1:B:41:TRP:CE3	1:B:105:VAL:HG21	2.18	0.79
1:A:281:GLY:HA3	1:A:284:LEU:HD22	1.65	0.78
1:B:206:LEU:HD23	1:B:299:PHE:HE1	1.47	0.78
1:A:20:ALA:HB3	1:A:31:PHE:CE1	2.18	0.77
1:B:47:CYS:HB2	1:B:106:ILE:HA	1.67	0.76
1:B:247:THR:HG21	1:B:254:LEU:HD21	1.67	0.76
1:A:221:THR:HG23	1:A:292:LEU:HB3	1.69	0.74
1:B:222:VAL:HG23	1:B:299:PHE:CE2	2.21	0.74
1:A:254:LEU:HD13	1:A:274:LEU:HD11	1.66	0.74
1:A:6:ILE:HD11	1:A:93:VAL:CG1	2.18	0.73
1:B:20:ALA:HB3	1:B:31:PHE:HE2	1.51	0.73
1:B:49:THR:HG21	1:B:108:THR:OG1	1.89	0.73
1:A:236:VAL:HG22	1:A:247:THR:HG23	1.73	0.70
1:B:78:VAL:HG22	2:D:352:STA:HD21	1.73	0.70
1:B:164:HIS:HD2	1:B:327:LYS:HG3	1.56	0.70
1:B:223:PRO:HG2	1:B:226:PHE:HB2	1.73	0.70
1:B:2:SER:HB3	1:B:148:LYS:O	1.92	0.69
1:B:6:ILE:HD11	1:B:93:VAL:HG12	1.74	0.69
1:B:44:SER:HB3	1:B:106:ILE:HG22	1.75	0.68
1:B:26:GLN:OE1	1:B:28:PRO:HD3	1.93	0.68
1:A:6:ILE:HD12	1:A:168:LEU:HD23	1.77	0.67
1:B:144:LYS:HA	1:B:149:ILE:HG22	1.76	0.67
1:A:155:THR:HG23	1:A:310:PHE:CE1	2.30	0.67
1:A:75:MET:HB3	1:A:82:VAL:HG12	1.78	0.66
1:B:206:LEU:HD23	1:B:299:PHE:CE1	2.31	0.65
1:B:188:ASN:HB2	1:B:194:GLN:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PHE:CZ	1:A:300:ILE:HD11	2.31	0.65
1:A:155:THR:HB	1:A:169:THR:HB	1.79	0.65
1:A:290:ILE:HG13	2:C:347:IVA:HG11	1.79	0.65
1:B:275:GLN:O	1:B:285:CYS:HB2	1.97	0.65
1:A:137:ASP:HB3	1:A:142:GLU:HG2	1.79	0.64
1:B:23:GLY:HA2	1:B:89:ASP:OD1	1.96	0.64
1:B:242:LEU:HB3	1:B:244:PHE:CD2	2.33	0.64
1:A:86:PHE:CD1	1:A:101:LYS:HE2	2.33	0.63
1:A:60:SER:HB2	1:A:66:TYR:CD2	2.33	0.63
1:A:21:GLU:HB2	1:A:26:GLN:O	1.98	0.63
1:A:251:ASN:ND2	1:A:253:LYS:H	1.96	0.63
1:A:82:VAL:HG22	1:A:105:VAL:HG11	1.80	0.63
1:A:214:ASP:O	1:A:302:GLY:HA2	1.97	0.63
1:B:88:LYS:HE2	1:B:99:PRO:HB3	1.81	0.63
1:B:24:ASP:OD2	1:B:64:ARG:HG2	2.00	0.62
1:B:277:ILE:HG13	1:B:286:MET:HE3	1.82	0.62
1:A:123:ILE:HD13	2:C:350:STA:HD11	1.81	0.61
1:A:128:TRP:HB2	1:A:191:LEU:O	2.00	0.61
1:B:25:ASN:HB2	1:B:62:LYS:O	1.99	0.61
1:A:60:SER:HB2	1:A:66:TYR:CG	2.34	0.61
1:B:242:LEU:HD13	1:B:244:PHE:CE2	2.35	0.61
1:A:174:GLU:HB3	1:A:176:ARG:HG2	1.83	0.60
1:B:149:ILE:HD11	1:B:170:ILE:O	2.00	0.60
1:A:29:PHE:HZ	1:A:58:TYR:HB2	1.67	0.60
1:A:66:TYR:HE1	1:A:87:SER:HB3	1.67	0.60
1:A:146:GLN:O	1:A:148:LYS:HG3	2.01	0.60
1:B:294:PHE:HZ	1:B:300:ILE:HD11	1.67	0.60
1:A:155:THR:HG23	1:A:310:PHE:HE1	1.67	0.59
1:B:160:VAL:HG22	1:B:307:ARG:HG2	1.84	0.59
1:A:217:THR:HA	2:C:348:VAL:O	2.02	0.59
1:B:6:ILE:O	1:B:167:PHE:HA	2.03	0.59
1:B:191:LEU:HB3	1:B:194:GLN:OE1	2.02	0.59
1:B:234:LEU:HG	1:B:236:VAL:HG13	1.84	0.58
1:B:277:ILE:HG22	1:B:280:VAL:HB	1.84	0.58
1:A:80:GLY:HA3	1:A:111:PHE:HD1	1.68	0.58
1:B:90:LEU:HA	1:B:99:PRO:HA	1.84	0.58
1:A:138:PRO:HB2	1:A:141:VAL:HB	1.86	0.58
1:B:49:THR:HG22	1:B:52:CYS:N	2.17	0.58
1:B:277:ILE:HG22	1:B:277:ILE:O	2.03	0.57
1:B:64:ARG:H	1:B:64:ARG:HD3	1.69	0.57
1:B:144:LYS:HD3	1:B:152:ALA:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:O	1:A:166:GLY:HA3	2.05	0.57
1:B:129:LYS:HE3	1:B:135:SER:HB2	1.86	0.57
1:B:155:THR:HG23	1:B:310:PHE:CE1	2.38	0.57
1:B:6:ILE:HB	1:B:168:LEU:HB3	1.87	0.57
1:A:247:THR:HG21	1:A:254:LEU:HD21	1.87	0.56
1:B:281:GLY:HA3	1:B:284:LEU:HD22	1.87	0.56
1:B:260:THR:HG22	1:B:265:LYS:HG3	1.87	0.56
1:B:9:VAL:O	1:B:16:PHE:HA	2.06	0.56
1:B:155:THR:O	1:B:168:LEU:HD12	2.06	0.56
1:B:69:ASP:HB3	1:B:86:PHE:O	2.06	0.56
1:B:270:PRO:HA	1:B:273:TYR:CZ	2.40	0.56
1:B:140:VAL:HB	1:B:315:TYR:HE2	1.71	0.56
1:B:25:ASN:O	1:B:26:GLN:HB3	2.06	0.56
1:A:231:LEU:HD23	1:A:234:LEU:HD12	1.88	0.56
1:A:188:ASN:ND2	1:A:194:GLN:HE21	2.02	0.56
1:B:22:VAL:O	1:B:27:GLN:HB2	2.06	0.56
1:A:198:ASP:O	1:A:259:PHE:HA	2.06	0.55
1:B:204:ILE:CD1	1:B:230:MET:HB3	2.36	0.55
1:B:43:PRO:HG2	1:B:56:HIS:O	2.07	0.55
1:B:204:ILE:HD11	1:B:230:MET:HA	1.88	0.55
1:B:273:TYR:HA	1:B:304:PRO:HB3	1.88	0.55
1:B:140:VAL:HB	1:B:315:TYR:CE2	2.42	0.55
1:A:258:GLU:HG3	1:A:267:THR:HG22	1.89	0.55
1:B:227:LEU:O	1:B:231:LEU:HG	2.06	0.55
1:A:160:VAL:HG11	1:A:163:LYS:HE3	1.88	0.54
1:B:242:LEU:HD13	1:B:244:PHE:HE2	1.72	0.54
1:A:3:ASN:HA	1:A:170:ILE:O	2.08	0.54
1:B:101:LYS:HD3	1:B:136:VAL:HG22	1.88	0.54
1:A:260:THR:HG22	1:A:265:LYS:HA	1.90	0.54
1:B:182:LEU:HD12	1:B:323:ALA:HB2	1.88	0.54
1:B:215:SER:HB3	1:B:306:MET:HE1	1.89	0.54
1:A:186:LYS:HD3	1:A:318:HIS:O	2.09	0.53
1:B:47:CYS:CB	1:B:106:ILE:HA	2.37	0.53
1:B:155:THR:CG2	1:B:156:PHE:N	2.72	0.53
1:A:78:VAL:HG22	2:C:352:STA:HD21	1.89	0.53
1:B:214:ASP:O	1:B:302:GLY:HA2	2.08	0.53
1:A:273:TYR:O	1:A:288:ASN:HB3	2.09	0.53
1:B:40:LEU:HD13	1:B:124:LEU:HG	1.91	0.53
1:A:21:GLU:HG2	1:A:92:THR:HB	1.91	0.52
1:B:222:VAL:CG1	1:B:227:LEU:HB2	2.39	0.52
1:B:2:SER:HB2	1:B:149:ILE:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ILE:CG2	1:B:280:VAL:HB	2.40	0.52
1:B:98:LEU:HD13	1:B:143:LEU:HD23	1.92	0.51
1:B:222:VAL:HG22	1:B:226:PHE:HB3	1.91	0.51
1:B:222:VAL:O	1:B:291:GLY:HA2	2.10	0.51
1:A:188:ASN:HD21	1:A:194:GLN:HE21	1.58	0.51
1:B:204:ILE:HD13	1:B:230:MET:HB3	1.91	0.51
1:A:45:VAL:HG23	1:A:58:TYR:O	2.10	0.51
1:A:14:ILE:HD11	1:A:275:GLN:CD	2.36	0.51
1:A:228:ASN:O	1:A:232:GLN:HG2	2.10	0.51
1:B:223:PRO:HG2	1:B:226:PHE:CB	2.39	0.51
1:A:163:LYS:HD2	1:A:164:HIS:CD2	2.46	0.50
2:D:348:VAL:HG11	2:D:350:STA:HD23	1.92	0.50
1:B:10:ASP:HB2	1:B:159:PRO:HG2	1.92	0.50
1:A:273:TYR:HE1	1:A:287:LEU:HD13	1.77	0.50
1:B:13:ASN:CG	1:B:161:HIS:HB2	2.36	0.50
1:B:303:ASP:HB3	1:B:307:ARG:NH1	2.27	0.50
1:A:141:VAL:HG23	1:A:315:TYR:CD2	2.47	0.50
1:B:16:PHE:CD2	1:B:158:LEU:HD22	2.46	0.50
1:B:33:LEU:HD23	1:B:124:LEU:HB3	1.94	0.50
1:B:144:LYS:CA	1:B:149:ILE:HG22	2.40	0.49
1:B:86:PHE:HD1	1:B:102:PHE:O	1.95	0.49
1:B:203:ASN:C	1:B:205:MET:SD	2.96	0.49
1:A:201:VAL:HG23	1:A:226:PHE:HZ	1.77	0.49
1:A:163:LYS:HD2	1:A:164:HIS:HD2	1.78	0.49
1:A:294:PHE:HZ	1:A:300:ILE:HD11	1.78	0.49
1:B:173:ILE:HD11	1:B:312:VAL:HG11	1.95	0.49
1:A:29:PHE:CZ	1:A:58:TYR:HB2	2.48	0.49
1:A:67:GLU:HB2	1:A:88:LYS:HB3	1.95	0.49
1:B:72:LYS:HD2	1:B:72:LYS:N	2.28	0.49
1:B:163:LYS:HB3	1:B:327:LYS:HG3	1.94	0.49
1:B:217:THR:HG23	2:D:349:VAL:HG22	1.93	0.49
1:B:21:GLU:HB2	1:B:26:GLN:O	2.13	0.49
1:B:49:THR:HG22	1:B:51:GLY:N	2.28	0.49
1:B:73:VAL:HG12	1:B:74:GLU:H	1.78	0.48
1:B:277:ILE:HB	1:B:285:CYS:HA	1.94	0.48
1:A:1:SER:C	1:A:3:ASN:H	2.20	0.48
1:B:274:LEU:HD13	1:B:285:CYS:SG	2.54	0.48
1:B:32:ILE:HB	1:B:123:ILE:HG12	1.96	0.47
1:A:80:GLY:HA3	1:A:111:PHE:CD1	2.48	0.47
1:A:273:TYR:CE1	1:A:287:LEU:HD13	2.48	0.47
1:B:175:GLU:HA	1:B:178:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD12	1:A:153:LEU:O	2.14	0.47
1:A:313:PHE:CD1	1:A:313:PHE:N	2.81	0.47
1:B:4:ASP:OD1	1:B:96:LEU:HG	2.14	0.47
1:B:73:VAL:HG12	1:B:74:GLU:N	2.29	0.47
1:B:140:VAL:HG21	1:B:154:PHE:CD2	2.49	0.47
1:A:201:VAL:HG12	1:A:255:PRO:HB2	1.95	0.47
1:A:137:ASP:CB	1:A:142:GLU:HG2	2.45	0.47
1:A:260:THR:HG22	1:A:265:LYS:HG3	1.97	0.47
1:A:303:ASP:O	1:A:307:ARG:HB2	2.14	0.47
1:B:92:THR:OG1	1:B:97:SER:HB2	2.15	0.47
1:B:155:THR:HG23	1:B:156:PHE:N	2.29	0.47
1:B:4:ASP:HB2	1:B:94:GLY:HA3	1.96	0.47
1:B:15:MET:HG3	1:B:16:PHE:H	1.79	0.47
1:B:290:ILE:HD11	2:D:347:IVA:HG21	1.97	0.47
1:A:174:GLU:OE1	1:A:176:ARG:HD3	2.14	0.47
1:B:153:LEU:HD12	1:B:153:LEU:O	2.15	0.47
1:A:40:LEU:O	1:A:103:ILE:HD12	2.15	0.46
1:A:201:VAL:HG23	1:A:226:PHE:CZ	2.50	0.46
1:A:201:VAL:CG1	1:A:255:PRO:HB2	2.45	0.46
1:B:15:MET:HG3	1:B:16:PHE:N	2.30	0.46
1:A:251:ASN:C	1:A:251:ASN:HD22	2.22	0.46
1:A:221:THR:CG2	1:A:292:LEU:HB3	2.41	0.46
1:A:41:TRP:CD1	1:A:77:TYR:HH	2.32	0.46
1:B:24:ASP:OD2	1:B:65:THR:HG23	2.15	0.46
1:A:144:LYS:O	1:A:145:ASN:C	2.59	0.46
1:B:10:ASP:OD1	1:B:13:ASN:HA	2.16	0.46
1:B:27:GLN:OE1	1:B:58:TYR:CD1	2.69	0.46
1:B:77:TYR:CB	2:D:350:STA:HD13	2.46	0.46
1:B:272:TYR:CD1	1:B:308:LYS:HB2	2.50	0.46
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.71	0.46
1:B:100:TYR:CE1	1:B:139:ILE:HG12	2.51	0.45
1:B:164:HIS:HD2	1:B:327:LYS:CG	2.25	0.45
1:A:188:ASN:HD22	1:A:189:HIS:CD2	2.33	0.45
1:B:51:GLY:O	1:B:54:THR:HB	2.15	0.45
1:B:47:CYS:SG	1:B:49:THR:HB	2.56	0.45
1:B:273:TYR:O	1:B:288:ASN:HB3	2.16	0.45
1:B:64:ARG:H	1:B:64:ARG:CD	2.28	0.45
1:B:70:GLY:N	1:B:86:PHE:O	2.50	0.45
1:B:303:ASP:O	1:B:307:ARG:N	2.46	0.45
1:A:49:THR:HG22	1:A:51:GLY:H	1.82	0.45
1:A:55:LYS:HG3	1:A:115:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:HD22	1:A:236:VAL:HG11	1.98	0.44
1:B:294:PHE:CZ	1:B:300:ILE:HD11	2.50	0.44
1:B:5:ASN:HB3	1:B:167:PHE:CD1	2.53	0.44
1:B:277:ILE:HG13	1:B:286:MET:CE	2.46	0.44
1:B:34:ASP:OD2	2:D:350:STA:HC	2.17	0.44
1:A:146:GLN:O	1:A:148:LYS:N	2.51	0.44
1:B:140:VAL:HG21	1:B:154:PHE:HD2	1.83	0.44
1:A:55:LYS:HE3	1:A:115:TYR:CE1	2.52	0.44
1:A:8:LEU:HD13	1:A:16:PHE:CE1	2.53	0.44
1:B:55:LYS:HG3	1:B:115:TYR:CZ	2.52	0.44
1:A:95:ASN:OD1	1:A:95:ASN:C	2.60	0.44
1:A:94:GLY:O	1:A:95:ASN:HB3	2.18	0.44
1:B:2:SER:CB	1:B:149:ILE:HA	2.48	0.44
1:B:41:TRP:HB2	1:B:105:VAL:CG2	2.48	0.44
1:B:77:TYR:HB3	2:D:350:STA:HA	2.00	0.44
1:B:220:ILE:HD13	1:B:220:ILE:HA	1.82	0.44
1:A:146:GLN:HB3	1:A:148:LYS:NZ	2.33	0.43
1:A:274:LEU:HD22	1:A:285:CYS:HB3	1.99	0.43
1:A:287:LEU:HD12	1:A:289:ILE:HD12	1.99	0.43
1:A:44:SER:OG	1:A:46:LYS:HD3	2.18	0.43
1:A:68:LYS:HB2	1:A:68:LYS:HE3	1.51	0.43
1:A:260:THR:CG2	1:A:265:LYS:HG3	2.48	0.43
1:B:228:ASN:HA	1:B:231:LEU:HD12	1.99	0.43
1:A:201:VAL:HG21	1:A:226:PHE:HE1	1.81	0.43
1:B:25:ASN:O	1:B:26:GLN:CB	2.65	0.43
1:A:65:THR:HG22	1:A:65:THR:O	2.17	0.43
1:A:251:ASN:HD22	1:A:252:SER:N	2.16	0.43
1:B:9:VAL:HG12	1:B:17:TYR:O	2.19	0.43
1:A:97:SER:O	1:A:148:LYS:HE2	2.19	0.43
1:B:200:HIS:HB2	1:B:258:GLU:HB2	1.99	0.43
2:D:352:STA:HD22	2:D:352:STA:HA	1.79	0.43
1:A:69:ASP:HB3	1:A:86:PHE:O	2.19	0.43
1:A:74:GLU:HG3	1:A:81:THR:CG2	2.49	0.43
1:B:44:SER:CB	1:B:104:GLU:HG2	2.35	0.43
1:B:67:GLU:CD	1:B:88:LYS:HD3	2.43	0.43
1:B:26:GLN:O	1:B:27:GLN:C	2.61	0.43
1:B:108:THR:HG21	1:B:115:TYR:CE2	2.53	0.43
1:A:294:PHE:CE1	1:A:300:ILE:HD11	2.53	0.43
1:B:22:VAL:HG22	1:B:91:VAL:HG22	2.01	0.43
1:A:22:VAL:HG12	1:A:23:GLY:N	2.34	0.43
1:A:230:MET:HE3	1:A:255:PRO:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HD12	1:B:248:LEU:HA	1.89	0.43
1:B:253:LYS:HA	1:B:253:LYS:HD3	1.73	0.43
1:B:17:TYR:CE1	1:B:120:PHE:HB3	2.54	0.42
1:B:201:VAL:HG13	1:B:255:PRO:HB2	2.01	0.42
1:B:225:ASP:CG	1:B:226:PHE:N	2.76	0.42
1:B:144:LYS:HE3	1:B:151:ASN:HA	2.00	0.42
1:A:91:VAL:HG21	1:A:100:TYR:HB3	2.01	0.42
1:B:51:GLY:O	1:B:55:LYS:HG2	2.19	0.42
1:B:55:LYS:HG3	1:B:115:TYR:OH	2.19	0.42
1:B:153:LEU:HD12	1:B:153:LEU:C	2.44	0.42
1:B:182:LEU:HD12	1:B:323:ALA:CB	2.49	0.42
1:B:182:LEU:HA	1:B:323:ALA:HB2	2.01	0.42
1:B:275:GLN:C	1:B:285:CYS:HB2	2.42	0.42
1:A:91:VAL:CG2	1:A:100:TYR:HB3	2.49	0.42
1:A:119:THR:O	1:A:119:THR:HG22	2.19	0.42
1:B:215:SER:HB3	1:B:306:MET:SD	2.58	0.42
1:B:34:ASP:O	1:B:126:LEU:N	2.52	0.42
1:B:137:ASP:HA	1:B:138:PRO:HD2	1.62	0.42
1:A:227:LEU:HD11	1:A:231:LEU:HD11	2.02	0.42
1:B:3:ASN:HA	1:B:170:ILE:O	2.19	0.42
1:B:55:LYS:HD2	1:B:120:PHE:O	2.19	0.42
1:B:222:VAL:HG21	1:B:226:PHE:CD1	2.55	0.42
1:A:149:ILE:O	1:A:149:ILE:HG13	2.20	0.42
1:A:157:TYR:HD2	1:A:166:GLY:HA2	1.84	0.42
1:A:275:GLN:HB2	1:A:286:MET:HG3	2.02	0.42
1:B:175:GLU:O	1:B:175:GLU:HG2	2.20	0.41
1:A:108:THR:HG21	1:A:115:TYR:CE2	2.55	0.41
1:A:145:ASN:C	1:A:147:ASN:H	2.27	0.41
1:A:153:LEU:HD12	1:A:153:LEU:C	2.45	0.41
1:A:155:THR:CG2	1:A:310:PHE:HE1	2.31	0.41
1:B:290:ILE:HG13	2:D:347:IVA:HG11	2.02	0.41
1:B:11:PHE:O	1:B:13:ASN:N	2.54	0.41
1:B:184:TYR:HD1	1:B:319:SER:HB3	1.85	0.41
1:B:270:PRO:HA	1:B:273:TYR:CE2	2.56	0.41
1:B:303:ASP:O	1:B:304:PRO:C	2.64	0.41
1:A:160:VAL:O	1:A:161:HIS:C	2.62	0.41
1:B:129:LYS:HD2	1:B:137:ASP:OD2	2.21	0.41
1:A:294:PHE:HB3	1:A:295:PRO:CD	2.51	0.41
1:B:278:GLU:OE2	1:B:282:PRO:HA	2.21	0.41
1:A:16:PHE:CE2	1:A:158:LEU:HD22	2.56	0.41
1:B:27:GLN:OE1	1:B:58:TYR:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASP:HB3	1:B:86:PHE:C	2.45	0.41
1:B:78:VAL:HG12	1:B:78:VAL:O	2.21	0.41
1:B:194:GLN:H	1:B:194:GLN:HG2	1.72	0.41
1:A:83:SER:O	1:A:105:VAL:HG13	2.21	0.41
1:A:221:THR:HB	1:A:300:ILE:CB	2.41	0.41
1:A:221:THR:HG21	1:A:292:LEU:HD23	2.02	0.41
1:B:6:ILE:CD1	1:B:93:VAL:HG12	2.47	0.41
1:B:113:PRO:O	1:B:114:THR:C	2.62	0.41
1:B:144:LYS:CB	1:B:152:ALA:HB2	2.50	0.41
1:B:303:ASP:O	1:B:306:MET:N	2.54	0.41
1:A:124:LEU:HD23	1:A:124:LEU:C	2.46	0.41
1:A:234:LEU:HA	1:A:253:LYS:HD2	2.02	0.41
1:B:100:TYR:CZ	1:B:139:ILE:HG12	2.56	0.41
1:A:188:ASN:O	1:A:189:HIS:CG	2.74	0.40
1:B:277:ILE:HD13	1:B:277:ILE:HA	1.68	0.40
1:B:230:MET:HE3	1:B:255:PRO:HG3	2.04	0.40
1:A:22:VAL:HG11	1:A:102:PHE:CE2	2.56	0.40
1:B:290:ILE:CD1	2:D:347:IVA:HG21	2.51	0.40
2:C:351:ALA:C	2:C:352:STA:HM2	2.47	0.40
1:A:29:PHE:HB2	1:A:31:PHE:CE1	2.57	0.40
1:A:278:GLU:O	1:A:278:GLU:HG3	2.21	0.40
1:B:294:PHE:HB2	1:B:296:VAL:O	2.22	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	327/329 (99%)	289 (88%)	30 (9%)	8 (2%)	4	12
1	B	327/329 (99%)	288 (88%)	29 (9%)	10 (3%)	3	8
2	C	3/6 (50%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	3/6 (50%)	3 (100%)	0	0	100	100
All	All	660/670 (98%)	583 (88%)	59 (9%)	18 (3%)	4	10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	161	HIS
1	B	161	HIS
1	A	69	ASP
1	A	147	ASN
1	A	297	PRO
1	B	12	GLN
1	B	49	THR
1	A	4	ASP
1	B	25	ASN
1	B	26	GLN
1	B	61	SER
1	B	70	GLY
1	A	5	ASN
1	A	162	ASP
1	B	27	GLN
1	B	138	PRO
1	B	297	PRO

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	294/294 (100%)	264 (90%)	30 (10%)	7	18
1	B	294/294 (100%)	264 (90%)	30 (10%)	7	18
2	C	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100
All	All	592/592 (100%)	532 (90%)	60 (10%)	7	18

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	21	GLU
1	A	24	ASP
1	A	42	VAL
1	A	45	VAL
1	A	46	LYS
1	A	71	THR
1	A	73	VAL
1	A	82	VAL
1	A	98	LEU
1	A	129	LYS
1	A	136	VAL
1	A	137	ASP
1	A	141	VAL
1	A	147	ASN
1	A	150	GLU
1	A	155	THR
1	A	158	LEU
1	A	165	THR
1	A	174	GLU
1	A	206	LEU
1	A	247	THR
1	A	252	SER
1	A	269	GLU
1	A	271	GLU
1	A	284	LEU
1	A	287	LEU
1	A	297	PRO
1	A	313	PHE
1	A	329	LEU
1	B	2	SER
1	B	4	ASP
1	B	6	ILE
1	B	14	ILE
1	B	21	GLU
1	B	32	ILE
1	B	60	SER
1	B	64	ARG
1	B	90	LEU
1	B	93	VAL
1	B	97	SER
1	B	112	GLU

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Mol	Chain	Res	Type
1	B	137	ASP
1	B	142	GLU
1	B	149	ILE
1	B	155	THR
1	B	174	GLU
1	B	187	LEU
1	B	194	GLN
1	B	198	ASP
1	B	205	MET
1	B	225	ASP
1	B	233	ASN
1	B	279	ASP
1	B	282	PRO
1	B	284	LEU
1	B	288	ASN
1	B	307	ARG
1	B	326	LYS
1	B	328	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	194	GLN
1	A	233	ASN
1	A	251	ASN
1	A	275	GLN
1	B	3	ASN
1	B	5	ASN
1	B	25	ASN
1	B	200	HIS
1	B	275	GLN
1	B	288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	STA	C	352	2	11,11,11	2.06	3 (27%)	11,14,14	1.51	3 (27%)
2	STA	D	350	2	10,10,11	1.59	2 (20%)	9,12,14	1.70	2 (22%)
2	STA	C	350	2	10,10,11	0.95	1 (10%)	9,12,14	1.32	1 (11%)
2	STA	D	352	2	11,11,11	1.15	1 (9%)	11,14,14	1.34	2 (18%)

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	STA	C	352	2	-	0/12/12/12	-
2	STA	D	350	2	-	3/11/11/12	-
2	STA	C	350	2	-	3/11/11/12	-
2	STA	D	352	2	-	0/12/12/12	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	352	STA	CH-CA	4.58	1.57	1.53
2	D	350	STA	CH-CA	3.94	1.57	1.53
2	C	352	STA	OH-CH	3.88	1.51	1.43
2	C	352	STA	OXT-C	-3.04	1.20	1.30
2	D	352	STA	OXT-C	-2.82	1.21	1.30
2	C	350	STA	CH-CA	2.74	1.56	1.53
2	D	350	STA	OH-CH	2.69	1.49	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	350	STA	CG-CB-CA	3.78	123.90	115.76
2	C	350	STA	OH-CH-CM	-3.11	102.09	109.24
2	C	352	STA	CM-CH-CA	-2.66	108.83	112.93
2	D	352	STA	OXT-C-O	-2.57	116.72	123.33
2	D	352	STA	OXT-C-CM	2.49	121.74	114.00
2	D	350	STA	CD2-CG-CD1	-2.43	99.69	110.53
2	C	352	STA	OH-CH-CM	2.38	115.18	109.45
2	C	352	STA	O-C-CM	-2.07	116.49	122.84

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	350	STA	N-CA-CB-CG
2	D	350	STA	N-CA-CB-CG
2	C	350	STA	CA-CH-CM-C
2	D	350	STA	CH-CA-CB-CG
2	C	350	STA	O-C-CM-CH
2	D	350	STA	O-C-CM-CH

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	352	STA	2	0
2	D	350	STA	4	0
2	C	350	STA	1	0
2	D	352	STA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.