



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:55 AM UTC

PDB ID : 5VAE / pdb\_00005vae  
Title : Crystal structure of accessory secretion protein 1 and 3  
Authors : Chen, Y.; Rapoport, T.A.; Jeffrey, P.D.  
Deposited on : 2017-03-25  
Resolution : 3.11 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](mailto: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>.

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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)  
Xtrriage (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

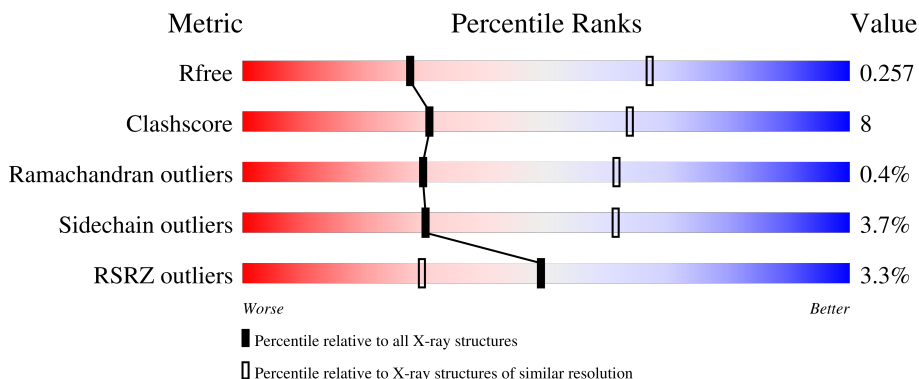
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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  $\geq 3$ , 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	533	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      76%      20%      ..</p>
1	C	533	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      74%      20%      ..</p>
1	E	533	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      74%      20%      ..</p>
1	G	533	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5%      71%      24%      ..</p>
2	B	159	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7%      62%      20%      ..      16%</p>

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Mol	Chain	Length	Quality of chain
2	D	159	
2	F	159	
2	H	159	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 21840 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 Accessory Sec system protein Asp1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	517	4350	2813	716	812	3	6	0	0	0
1	C	513	4317	2792	710	806	3	6	0	0	0
1	E	510	4294	2780	707	798	3	6	0	0	0
1	G	510	4291	2778	706	798	3	6	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	527	VAL	-	expression tag	UNP Q9AET9
A	528	ASP	-	expression tag	UNP Q9AET9
A	529	LYS	-	expression tag	UNP Q9AET9
A	530	LEU	-	expression tag	UNP Q9AET9
A	531	VAL	-	expression tag	UNP Q9AET9
A	532	PRO	-	expression tag	UNP Q9AET9
A	533	ARG	-	expression tag	UNP Q9AET9
C	527	VAL	-	expression tag	UNP Q9AET9
C	528	ASP	-	expression tag	UNP Q9AET9
C	529	LYS	-	expression tag	UNP Q9AET9
C	530	LEU	-	expression tag	UNP Q9AET9
C	531	VAL	-	expression tag	UNP Q9AET9
C	532	PRO	-	expression tag	UNP Q9AET9
C	533	ARG	-	expression tag	UNP Q9AET9
E	527	VAL	-	expression tag	UNP Q9AET9
E	528	ASP	-	expression tag	UNP Q9AET9
E	529	LYS	-	expression tag	UNP Q9AET9
E	530	LEU	-	expression tag	UNP Q9AET9
E	531	VAL	-	expression tag	UNP Q9AET9
E	532	PRO	-	expression tag	UNP Q9AET9
E	533	ARG	-	expression tag	UNP Q9AET9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	527	VAL	-	expression tag	UNP Q9AET9
G	528	ASP	-	expression tag	UNP Q9AET9
G	529	LYS	-	expression tag	UNP Q9AET9
G	530	LEU	-	expression tag	UNP Q9AET9
G	531	VAL	-	expression tag	UNP Q9AET9
G	532	PRO	-	expression tag	UNP Q9AET9
G	533	ARG	-	expression tag	UNP Q9AET9

- Molecule 2 is a protein called Accessory Sec system protein Asp3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	134	1126	724	188	210	1	3	0	0	0
2	D	134	1126	724	188	210	1	3	0	0	0
2	F	134	1126	724	188	210	1	3	0	0	0
2	H	134	1126	724	188	210	1	3	0	0	0

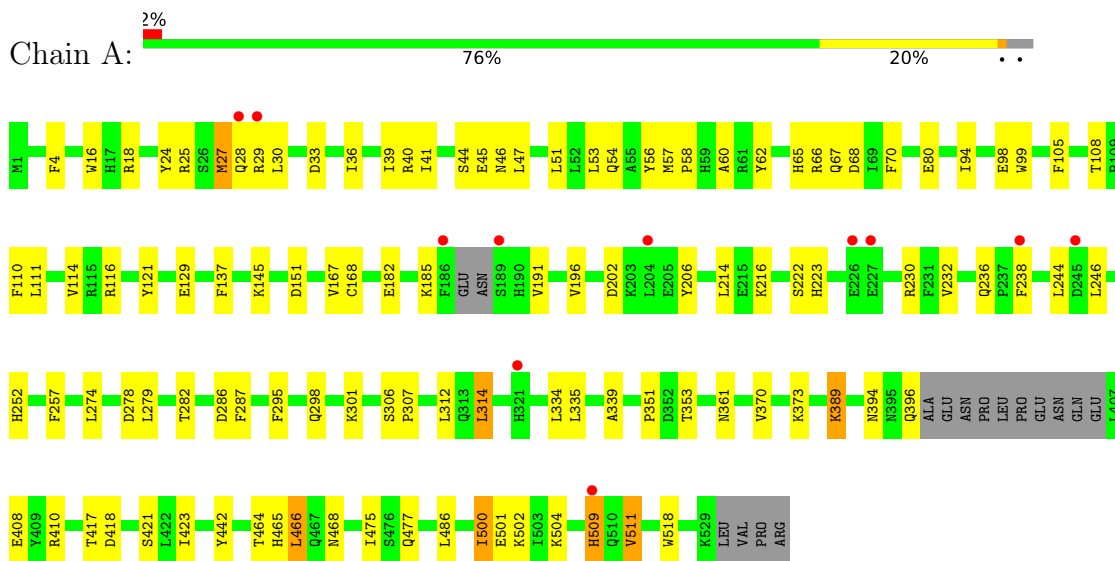
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total 26	O 26	0	0
3	B	2	Total 2	O 2	0	0
3	C	19	Total 19	O 19	0	0
3	D	3	Total 3	O 3	0	0
3	E	17	Total 17	O 17	0	0
3	F	1	Total 1	O 1	0	0
3	G	14	Total 14	O 14	0	0
3	H	2	Total 2	O 2	0	0

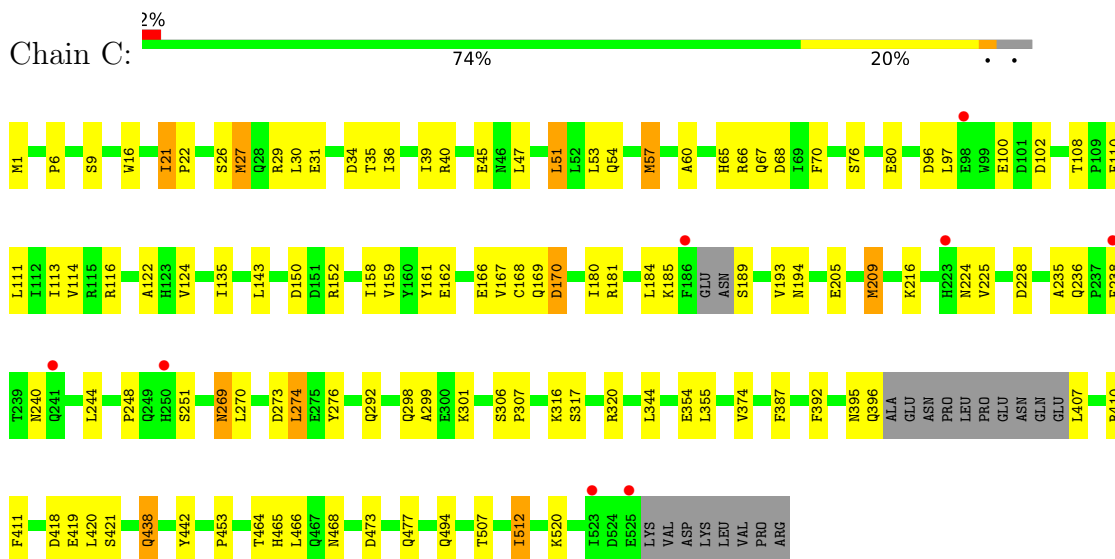
### 3 Residue-property plots i

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: Accessory Sec system protein Asp1

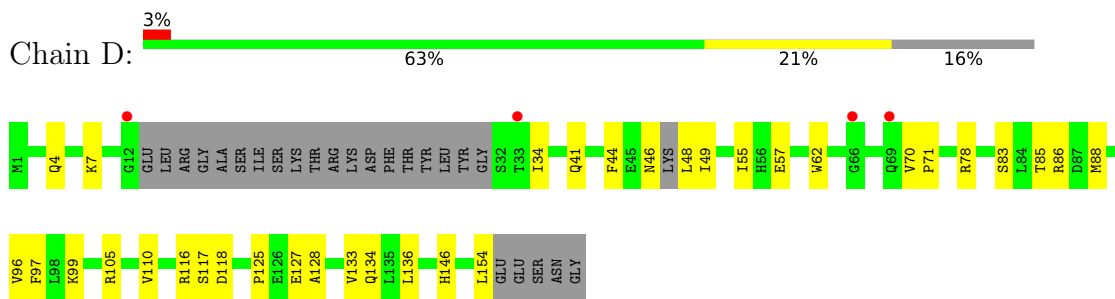


- Molecule 1: Accessory Sec system protein Asp1

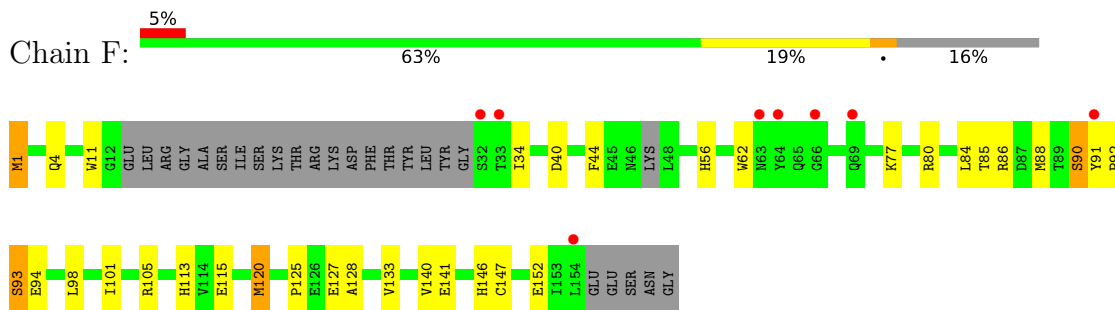


- Molecule 1: Accessory Sec system protein Asp1

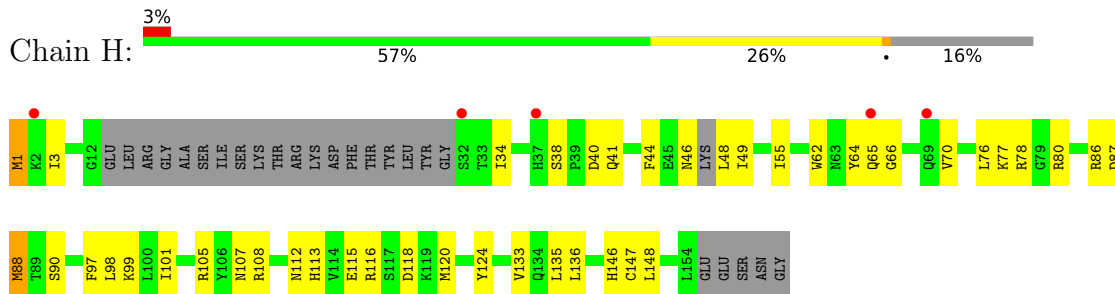




- Molecule 2: Accessory Sec system protein Asp3



- Molecule 2: Accessory Sec system protein Asp3



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.60Å 257.29Å 217.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 3.11 49.90 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.90-3.11) 99.5 (49.90-3.11)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.207 , 0.248 0.215 , 0.257	Depositor DCC
$R_{free}$ test set	3863 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 26.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	21840	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.62	1/4453 (0.0%)	0.91	5/6022 (0.1%)
1	C	0.66	0/4420	0.96	8/5979 (0.1%)
1	E	0.64	0/4397	0.94	4/5948 (0.1%)
1	G	0.58	0/4394	0.91	8/5944 (0.1%)
2	B	0.57	1/1154 (0.1%)	0.89	5/1553 (0.3%)
2	D	0.65	0/1154	0.87	1/1553 (0.1%)
2	F	0.60	1/1154 (0.1%)	0.90	4/1553 (0.3%)
2	H	0.62	1/1154 (0.1%)	0.87	1/1553 (0.1%)
All	All	0.62	4/22280 (0.0%)	0.92	36/30105 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	MSE	SE-CE	-6.24	1.76	1.95
1	A	238	PHE	CA-C	5.95	1.55	1.52
2	H	1	MSE	SE-CE	-5.15	1.79	1.95
2	B	1	MSE	SE-CE	-5.15	1.80	1.95

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	332	SER	N-CA-C	-10.36	99.52	112.88
1	A	44	SER	N-CA-C	-7.72	99.70	110.35
1	A	509	HIS	N-CA-C	-7.71	102.87	111.82
1	G	242	GLY	N-CA-C	-7.64	103.92	112.33
2	B	147	CYS	N-CA-C	6.99	117.74	107.88
2	D	110	VAL	N-CA-C	-6.92	106.05	112.96
2	H	147	CYS	N-CA-C	6.88	117.67	108.38
1	A	236	GLN	CA-C-N	6.78	128.31	119.84
1	A	236	GLN	C-N-CA	6.78	128.31	119.84
2	F	91	TYR	CA-C-N	-6.60	113.01	121.91
2	F	91	TYR	C-N-CA	-6.60	113.01	121.91
1	C	224	ASN	N-CA-C	6.46	120.16	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	438	GLN	CA-C-N	6.34	126.29	119.76
1	C	438	GLN	C-N-CA	6.34	126.29	119.76
1	A	502	LYS	N-CA-C	-6.01	106.59	114.04
2	F	147	CYS	N-CA-C	5.79	116.94	108.14
1	C	209	MSE	CG-SE-CE	-5.70	86.39	98.92
1	E	185	LYS	N-CA-C	-5.65	104.61	113.02
2	F	93	SER	CB-CA-C	-5.61	110.09	116.54
1	G	108	THR	CA-C-N	-5.55	115.17	120.83
1	G	108	THR	C-N-CA	-5.55	115.17	120.83
1	G	438	GLN	CA-C-N	5.50	125.45	119.78
1	G	438	GLN	C-N-CA	5.50	125.45	119.78
1	E	46	ASN	N-CA-C	5.40	122.31	110.80
1	E	333	GLU	N-CA-C	-5.28	103.06	110.35
1	C	21	ILE	CA-C-N	5.24	125.52	119.92
1	C	21	ILE	C-N-CA	5.24	125.52	119.92
2	B	93	SER	CB-CA-C	-5.18	110.18	117.23
2	B	91	TYR	CA-C-N	-5.16	113.39	119.84
2	B	91	TYR	C-N-CA	-5.16	113.39	119.84
1	C	419	GLU	N-CA-C	-5.14	105.75	112.23
1	G	270	LEU	N-CA-C	-5.12	106.98	113.18
1	C	228	ASP	N-CA-C	-5.07	104.42	111.52
1	E	225	VAL	CB-CA-C	-5.07	105.76	111.23
2	B	65	GLN	N-CA-C	5.06	117.19	111.11
1	G	25	ARG	N-CA-C	-5.01	107.22	113.38

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4350	0	4224	63	0
1	C	4317	0	4185	66	0
1	E	4294	0	4170	72	0
1	G	4291	0	4167	82	0
2	B	1126	0	1084	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1126	0	1084	17	2
2	F	1126	0	1084	19	0
2	H	1126	0	1084	27	2
3	A	26	0	0	0	0
3	B	2	0	0	0	0
3	C	19	0	0	1	0
3	D	3	0	0	1	0
3	E	17	0	0	0	0
3	F	1	0	0	0	0
3	G	14	0	0	2	0
3	H	2	0	0	0	0
All	All	21840	0	21082	356	2

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 8.

All (356) 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:A:40:ARG:NH1	1:A:67:GLN:O	2.09	0.85
1:G:298:GLN:HB3	1:G:301:LYS:HE2	1.58	0.84
1:E:1:MSE:HE2	1:E:48:PRO:HB2	1.63	0.79
1:E:97:LEU:HB3	2:F:1:MSE:HE3	1.64	0.78
1:G:155:VAL:HG23	2:H:3:ILE:HD11	1.65	0.77
2:D:48:LEU:HD23	2:D:49:ILE:HG13	1.65	0.77
1:C:465:HIS:CD2	1:C:466:LEU:HG	2.19	0.77
1:G:31:GLU:OE2	1:G:66:ARG:NH1	2.19	0.76
1:G:30:LEU:HD13	1:G:442:TYR:HB2	1.68	0.76
1:A:41:ILE:HD13	1:A:511:VAL:HG11	1.68	0.75
1:G:347:VAL:O	1:G:410:ARG:NH2	2.19	0.75
1:C:235:ALA:HA	1:C:240:ASN:HD21	1.49	0.75
2:H:99:LYS:HE3	2:H:112:ASN:HD22	1.51	0.75
1:G:483:ASP:HB2	1:G:487:GLN:HG3	1.70	0.74
1:A:167:VAL:HG23	1:A:185:LYS:HD2	1.69	0.73
2:F:125:PRO:HG2	2:F:128:ALA:HB2	1.71	0.73
1:E:30:LEU:HD13	1:E:442:TYR:HB2	1.69	0.73
1:A:312:LEU:HD13	1:A:423:ILE:HG23	1.71	0.72
1:E:298:GLN:HG3	1:E:301:LYS:HE2	1.71	0.72
1:E:27:MSE:HE1	1:E:361:ASN:HA	1.72	0.72
1:A:51:LEU:HG	1:A:53:LEU:HD21	1.70	0.72
1:G:386:ASP:O	1:G:410:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:LYS:O	1:C:189:SER:HB2	1.91	0.70
1:E:18:ARG:HG3	1:E:57:MSE:HB3	1.74	0.70
1:C:31:GLU:OE2	1:C:66:ARG:NH1	2.27	0.68
2:H:115:GLU:HB2	2:H:120:MSE:HE2	1.76	0.68
1:C:270:LEU:HB3	1:C:274:LEU:HD12	1.75	0.68
1:E:96:ASP:HB2	2:F:4:GLN:HB2	1.75	0.67
2:F:115:GLU:HG3	2:F:120:MSE:HB2	1.77	0.67
1:C:68:ASP:OD1	2:D:105:ARG:NH2	2.28	0.66
1:E:282:THR:HG21	1:E:287:PHE:HB3	1.77	0.66
2:B:77:LYS:HB2	2:B:80:ARG:HD2	1.78	0.66
2:D:125:PRO:HG2	2:D:128:ALA:HB2	1.78	0.66
1:E:45:GLU:O	1:E:47:LEU:N	2.25	0.66
2:B:125:PRO:HG2	2:B:128:ALA:HB2	1.76	0.66
1:A:30:LEU:HD13	1:A:442:TYR:HB2	1.77	0.66
1:E:317:SER:HB2	1:E:430:ARG:HH11	1.61	0.65
1:C:96:ASP:HB2	2:D:4:GLN:HB2	1.78	0.65
1:E:108:THR:HB	1:E:111:LEU:H	1.62	0.64
2:H:86:ARG:NE	2:H:88:MSE:HE3	2.12	0.64
1:E:225:VAL:HG11	1:E:231:PHE:HZ	1.63	0.63
1:E:31:GLU:OE2	1:E:66:ARG:NH2	2.23	0.63
2:H:77:LYS:HB2	2:H:80:ARG:HD2	1.81	0.63
1:G:36:ILE:O	1:G:40:ARG:HG3	1.97	0.63
1:A:314:LEU:HD21	1:A:500:ILE:HD11	1.80	0.63
2:D:86:ARG:NH2	2:D:96:VAL:O	2.27	0.62
1:C:30:LEU:HD13	1:C:442:TYR:HB2	1.81	0.62
1:A:36:ILE:O	1:A:40:ARG:HG3	2.00	0.62
1:A:65:HIS:HA	1:A:70:PHE:HB2	1.80	0.62
1:C:36:ILE:O	1:C:40:ARG:HG3	2.00	0.62
1:C:108:THR:HG22	1:C:110:PHE:H	1.63	0.62
1:G:200:ASP:O	1:G:216:LYS:NZ	2.31	0.62
1:C:159:VAL:HG22	1:C:169:GLN:HB2	1.82	0.62
1:E:150:ASP:OD1	1:E:152:ARG:HD2	1.99	0.61
2:D:86:ARG:HE	2:D:88:MSE:HE3	1.65	0.61
1:A:33:ASP:HB3	1:A:36:ILE:HG13	1.83	0.61
1:A:116:ARG:HG2	1:A:121:TYR:HB2	1.83	0.61
1:C:6:PRO:HB3	1:C:35:THR:HG21	1.83	0.61
1:G:57:MSE:HB2	1:G:60:ALA:HB2	1.82	0.60
1:G:457:LEU:HD23	1:G:472:LEU:HB2	1.84	0.60
1:A:57:MSE:HB2	1:A:60:ALA:HB2	1.83	0.60
1:A:108:THR:HG22	1:A:110:PHE:H	1.65	0.60
1:E:457:LEU:HD11	1:E:475:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:THR:H	1:C:468:ASN:HB2	1.68	0.59
1:E:225:VAL:HG11	1:E:231:PHE:CZ	2.36	0.59
1:E:435:LEU:HD13	1:E:475:ILE:HD12	1.85	0.59
1:E:61:ARG:N	1:E:151:ASP:OD2	2.31	0.59
1:A:464:THR:H	1:A:468:ASN:HB2	1.68	0.59
2:B:86:ARG:HH11	2:B:98:LEU:HB2	1.67	0.58
1:C:114:VAL:HB	1:C:122:ALA:HB3	1.86	0.58
2:F:86:ARG:NE	2:F:88:MSE:HE2	2.18	0.58
1:G:427:ASP:OD2	2:H:108:ARG:NH2	2.36	0.58
1:G:194:ASN:OD1	1:G:196:VAL:HG13	2.04	0.58
1:G:40:ARG:NH1	1:G:67:GLN:O	2.35	0.58
1:A:56:TYR:CZ	1:A:58:PRO:HG3	2.39	0.57
2:B:84:LEU:HD23	2:B:120:MSE:HE3	1.86	0.57
1:C:51:LEU:HG	1:C:53:LEU:HD21	1.86	0.57
1:A:418:ASP:HB2	1:A:421:SER:H	1.68	0.57
1:E:464:THR:H	1:E:468:ASN:HB2	1.69	0.57
1:C:39:ILE:HD11	1:C:51:LEU:HD13	1.87	0.57
1:E:51:LEU:HG	1:E:53:LEU:HD21	1.88	0.56
1:C:473:ASP:HB2	1:C:477:GLN:OE1	2.05	0.56
1:A:39:ILE:HD11	1:A:51:LEU:HD13	1.87	0.56
1:C:65:HIS:HA	1:C:70:PHE:HB2	1.86	0.56
1:G:182:GLU:HG3	1:G:191:VAL:HG22	1.88	0.56
1:C:57:MSE:HB2	1:C:60:ALA:HB2	1.86	0.56
1:E:392:PHE:CE2	1:E:407:LEU:HA	2.41	0.56
1:E:317:SER:HB2	1:E:430:ARG:NH1	2.21	0.56
1:G:6:PRO:HB3	1:G:35:THR:HG21	1.87	0.56
2:B:38:SER:HB2	2:B:41:GLN:HG2	1.86	0.55
2:D:86:ARG:NE	2:D:88:MSE:HE3	2.21	0.55
2:H:105:ARG:C	2:H:107:ASN:H	2.14	0.55
2:B:86:ARG:NE	2:B:88:MSE:HE2	2.21	0.55
1:A:222:SER:HB2	1:A:223:HIS:CD2	2.42	0.55
2:B:92:PRO:HG3	2:B:141:GLU:H	1.72	0.55
1:E:15:VAL:HG11	1:E:238:PHE:HZ	1.72	0.55
1:E:418:ASP:HB2	1:E:421:SER:H	1.72	0.55
1:E:236:GLN:C	1:E:238:PHE:H	2.15	0.55
1:G:464:THR:H	1:G:468:ASN:HB2	1.71	0.55
1:E:473:ASP:HB2	1:E:477:GLN:HE22	1.70	0.55
1:E:40:ARG:NH1	1:E:67:GLN:O	2.38	0.55
1:G:521:GLU:OE2	1:G:521:GLU:N	2.40	0.55
1:E:61:ARG:HH21	1:E:151:ASP:HB2	1.71	0.55
2:D:86:ARG:HD3	2:D:118:ASP:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:ILE:O	1:E:504:LYS:HG2	2.07	0.54
1:E:1:MSE:HG2	1:E:2:TYR:N	2.22	0.54
1:E:236:GLN:HG3	1:E:238:PHE:CD2	2.41	0.54
1:E:56:TYR:OH	1:E:157:SER:HB2	2.07	0.54
1:G:312:LEU:HD13	1:G:423:ILE:HG23	1.90	0.54
1:A:298:GLN:HB3	1:A:301:LYS:HE3	1.90	0.54
1:G:217:LEU:O	1:G:221:ILE:HG13	2.08	0.54
1:G:335:LEU:HD21	1:G:370:VAL:HG22	1.90	0.54
1:E:65:HIS:HA	1:E:70:PHE:HB2	1.89	0.53
1:G:51:LEU:HG	1:G:53:LEU:CD1	2.39	0.53
1:A:66:ARG:NH1	1:A:129:GLU:OE2	2.42	0.53
1:A:353:THR:O	1:A:410:ARG:HD2	2.09	0.53
1:C:270:LEU:O	1:C:274:LEU:HB2	2.09	0.53
1:G:33:ASP:HB3	1:G:36:ILE:H	1.73	0.53
1:G:51:LEU:HG	1:G:53:LEU:HD11	1.89	0.53
1:A:501:GLU:HA	1:A:504:LYS:HE2	1.91	0.53
2:H:40:ASP:HB2	2:H:146:HIS:CE1	2.43	0.53
2:H:99:LYS:HD2	2:H:136:LEU:HD11	1.91	0.53
1:C:395:ASN:O	1:C:396:GLN:HG3	2.10	0.53
1:C:45:GLU:HB2	1:C:47:LEU:HG	1.91	0.52
1:C:344:LEU:HD21	1:C:374:VAL:HG13	1.90	0.52
1:G:292:GLN:HG2	1:G:299:ALA:HB1	1.91	0.52
2:F:77:LYS:HB2	2:F:80:ARG:HD2	1.92	0.52
2:D:78:ARG:NH1	3:D:201:HOH:O	2.34	0.52
1:G:68:ASP:CG	2:H:105:ARG:HH22	2.17	0.52
1:A:68:ASP:OD1	2:B:105:ARG:NH2	2.44	0.51
2:B:86:ARG:HD2	2:B:98:LEU:HB2	1.92	0.51
1:C:124:VAL:HG13	1:C:135:ILE:HG12	1.92	0.51
1:C:161:TYR:CE1	1:C:166:GLU:HG2	2.45	0.51
1:C:180:ILE:HD11	1:C:209:MSE:HE1	1.93	0.51
1:A:108:THR:HB	1:A:111:LEU:H	1.74	0.51
1:E:288:LYS:HG3	1:E:302:ILE:HG22	1.93	0.51
1:G:288:LYS:HG3	1:G:302:ILE:HG22	1.92	0.51
1:C:100:GLU:HG2	1:C:116:ARG:NH2	2.26	0.51
1:E:236:GLN:HG3	1:E:238:PHE:HD2	1.75	0.51
1:G:387:PHE:O	1:G:410:ARG:HG2	2.10	0.51
2:B:93:SER:OG	2:B:94:GLU:N	2.44	0.51
1:G:269:ASN:OD1	1:G:269:ASN:N	2.43	0.50
1:A:182:GLU:HG3	1:A:191:VAL:HG22	1.94	0.50
1:A:339:ALA:HA	1:A:475:ILE:HD12	1.93	0.50
1:C:392:PHE:CE2	1:C:407:LEU:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:SER:HB2	1:E:223:HIS:ND1	2.26	0.50
1:E:267:ILE:HG22	1:E:295:PHE:HE2	1.77	0.50
1:E:282:THR:HG22	1:E:284:ARG:H	1.77	0.50
2:H:1:MSE:HE2	2:H:1:MSE:HA	1.92	0.50
1:C:162:GLU:HG3	1:C:167:VAL:HG11	1.93	0.50
2:D:49:ILE:HD13	2:D:55:ILE:HA	1.94	0.50
1:E:320:ARG:NH2	1:E:354:GLU:OE1	2.43	0.50
1:G:108:THR:HB	1:G:111:LEU:H	1.75	0.50
1:C:418:ASP:HB2	1:C:421:SER:H	1.75	0.50
1:G:1:MSE:HG2	1:G:2:TYR:H	1.76	0.50
1:G:100:GLU:HG3	1:G:101:ASP:H	1.77	0.49
1:G:65:HIS:HA	1:G:70:PHE:HB2	1.93	0.49
1:C:108:THR:HB	1:C:111:LEU:H	1.77	0.49
1:C:40:ARG:NH1	1:C:67:GLN:O	2.42	0.49
1:C:418:ASP:HB3	1:C:420:LEU:H	1.77	0.49
1:G:352:ASP:OD1	1:G:390:LYS:NZ	2.27	0.49
2:B:76:LEU:HD22	2:B:131:TYR:CE1	2.48	0.49
1:G:150:ASP:OD1	1:G:152:ARG:NH1	2.46	0.49
1:E:79:ASP:OD2	1:E:152:ARG:NH2	2.45	0.49
2:H:98:LEU:HD23	2:H:120:MSE:HE3	1.94	0.49
2:F:80:ARG:HG3	2:F:80:ARG:HH11	1.77	0.48
1:G:1:MSE:CE	1:G:48:PRO:HB2	2.43	0.48
1:C:29:ARG:HG2	1:C:30:LEU:H	1.77	0.48
1:C:80:GLU:CD	1:C:216:LYS:HD2	2.38	0.48
1:G:16:TRP:CD1	1:G:16:TRP:H	2.31	0.48
1:G:31:GLU:CD	1:G:66:ARG:HH11	2.22	0.48
1:G:248:PRO:O	1:G:251:SER:OG	2.31	0.48
1:C:47:LEU:HD12	1:C:512:ILE:HD12	1.94	0.48
2:H:86:ARG:HD3	2:H:118:ASP:HA	1.95	0.48
1:C:236:GLN:C	1:C:238:PHE:H	2.22	0.48
1:E:27:MSE:CE	1:E:361:ASN:HA	2.41	0.48
1:G:390:LYS:C	1:G:392:PHE:H	2.21	0.48
1:C:244:LEU:HD22	1:C:276:TYR:HD2	1.77	0.48
1:G:337:ASP:CG	1:G:373:LYS:HE2	2.38	0.48
1:A:167:VAL:HG13	1:A:168:CYS:HB3	1.94	0.48
1:C:16:TRP:CD1	1:C:16:TRP:H	2.30	0.48
2:F:40:ASP:O	2:F:146:HIS:HA	2.13	0.48
1:G:39:ILE:HD11	1:G:51:LEU:HD13	1.96	0.48
1:G:191:VAL:HG21	1:G:209:MSE:HG2	1.96	0.48
1:G:473:ASP:HB2	1:G:477:GLN:HE22	1.78	0.48
2:F:93:SER:OG	2:F:94:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:PHE:HB2	1:G:189:SER:HB3	1.94	0.47
1:A:105:PHE:HD1	1:A:114:VAL:HG22	1.79	0.47
1:G:51:LEU:HD22	1:G:72:THR:HG21	1.96	0.47
1:G:459:ALA:HA	1:G:471:ILE:HD13	1.94	0.47
1:A:286:ASP:OD1	1:A:286:ASP:N	2.42	0.47
1:G:56:TYR:CZ	1:G:58:PRO:HG3	2.50	0.47
1:G:271:LYS:HG3	1:G:295:PHE:HE1	1.80	0.47
1:G:465:HIS:CE1	1:G:466:LEU:HG	2.50	0.47
2:H:87:ASP:OD2	2:H:146:HIS:HD2	1.98	0.47
1:A:16:TRP:CD1	1:A:16:TRP:H	2.31	0.47
1:G:428:ASP:OD1	1:G:428:ASP:N	2.48	0.47
1:E:337:ASP:OD1	1:E:373:LYS:HE3	2.15	0.47
1:G:116:ARG:HG2	1:G:121:TYR:HB2	1.97	0.47
2:H:34:ILE:HG13	2:H:44:PHE:HD1	1.79	0.47
1:C:244:LEU:HD22	1:C:276:TYR:CD2	2.50	0.47
1:G:238:PHE:CD2	1:G:239:THR:HG22	2.50	0.47
1:E:16:TRP:HH2	1:E:182:GLU:OE1	1.97	0.46
2:F:86:ARG:HD2	2:F:98:LEU:HB2	1.97	0.46
1:A:394:ASN:HB3	1:C:143:LEU:HB3	1.97	0.46
2:H:86:ARG:CZ	2:H:88:MSE:HE3	2.45	0.46
1:C:248:PRO:HB2	1:C:251:SER:HB3	1.96	0.46
1:C:298:GLN:HB3	1:C:301:LYS:HE2	1.96	0.46
1:E:36:ILE:O	1:E:40:ARG:HG3	2.16	0.46
2:F:84:LEU:HD23	2:F:120:MSE:HE3	1.96	0.46
1:A:477:GLN:HG3	1:C:438:GLN:OE1	2.16	0.46
1:C:269:ASN:N	1:C:269:ASN:OD1	2.48	0.46
1:G:210:PRO:HA	1:G:213:ILE:HB	1.98	0.46
1:C:453:PRO:HA	1:C:468:ASN:O	2.16	0.46
2:F:80:ARG:HD3	2:F:152:GLU:OE2	2.16	0.46
2:B:80:ARG:HG3	2:B:80:ARG:HH11	1.81	0.46
1:E:283:ASP:HB2	1:E:307:PRO:HD3	1.98	0.46
1:A:335:LEU:HD21	1:A:370:VAL:HG22	1.98	0.45
1:C:158:ILE:O	1:C:169:GLN:HA	2.16	0.45
1:G:140:ASP:C	1:G:142:GLN:H	2.24	0.45
1:E:8:TRP:HE3	1:E:57:MSE:HE1	1.80	0.45
1:E:312:LEU:HD13	1:E:423:ILE:HG23	1.97	0.45
1:A:24:TYR:CE1	1:A:25:ARG:HG3	2.51	0.45
1:C:168:CYS:SG	1:C:181:ARG:HD3	2.57	0.45
1:G:473:ASP:HB2	1:G:477:GLN:NE2	2.31	0.45
2:H:64:TYR:O	2:H:66:GLY:N	2.49	0.45
2:H:112:ASN:C	2:H:113:HIS:HD1	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HG3	1:A:57:MSE:HG2	1.99	0.45
1:A:24:TYR:CD1	1:A:25:ARG:HG3	2.52	0.45
1:A:27:MSE:HE1	1:A:361:ASN:HA	1.98	0.45
1:C:320:ARG:NH2	1:C:354:GLU:OE1	2.43	0.45
1:G:267:ILE:HG22	1:G:295:PHE:HE2	1.81	0.45
2:F:34:ILE:HG13	2:F:44:PHE:HD1	1.82	0.45
1:G:130:GLY:O	2:H:70:VAL:HG13	2.16	0.45
2:B:84:LEU:HD23	2:B:120:MSE:CE	2.47	0.45
1:C:520:LYS:HD2	1:C:520:LYS:HA	1.75	0.45
1:E:307:PRO:HD2	1:E:462:TYR:OH	2.17	0.45
1:G:392:PHE:CZ	1:G:407:LEU:HA	2.52	0.45
1:G:419:GLU:OE1	3:G:601:HOH:O	2.21	0.45
1:G:464:THR:H	1:G:468:ASN:CB	2.29	0.44
1:A:274:LEU:HD23	1:A:295:PHE:CD2	2.52	0.44
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.73	0.44
1:C:387:PHE:O	1:C:410:ARG:HG2	2.17	0.44
1:E:16:TRP:CD1	1:E:16:TRP:H	2.34	0.44
1:E:467:GLN:HB3	1:E:498:TYR:CD2	2.52	0.44
1:C:16:TRP:CH2	1:C:209:MSE:HG3	2.53	0.44
1:E:473:ASP:HB2	1:E:477:GLN:NE2	2.31	0.44
2:B:34:ILE:H	2:B:34:ILE:HG13	1.49	0.44
1:G:173:ASN:OD1	1:G:176:GLY:N	2.49	0.44
2:H:77:LYS:CB	2:H:80:ARG:HD2	2.48	0.44
1:A:202:ASP:O	1:A:206:TYR:OH	2.34	0.44
1:G:239:THR:C	1:G:241:GLN:H	2.25	0.44
1:E:453:PRO:HA	1:E:468:ASN:O	2.18	0.44
1:G:426:LEU:HD23	1:G:426:LEU:HA	1.79	0.43
1:A:214:LEU:HD21	1:A:246:LEU:HD11	2.00	0.43
1:E:226:GLU:HB3	1:E:227:GLU:HB3	2.00	0.43
1:E:239:THR:HG22	1:E:241:GLN:H	1.82	0.43
1:C:54:GLN:HG3	3:C:605:HOH:O	2.17	0.43
1:A:465:HIS:CE1	1:A:466:LEU:HD13	2.53	0.43
1:C:170:ASP:OD1	1:C:170:ASP:N	2.52	0.43
1:G:1:MSE:HE2	1:G:48:PRO:HB2	2.01	0.43
1:A:137:PHE:HB2	1:A:145:LYS:HB2	2.00	0.43
1:A:279:LEU:HD11	1:A:518:TRP:HB3	2.00	0.43
1:G:373:LYS:HA	1:G:373:LYS:HD2	1.71	0.43
1:E:371:GLU:HG2	1:E:413:ILE:HD12	2.01	0.43
2:B:95:SER:HB2	2:B:140:VAL:HG22	1.99	0.43
2:D:7:LYS:HE2	2:D:7:LYS:HB3	1.91	0.43
1:C:193:VAL:HG12	1:C:194:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:OE1	1:A:216:LYS:HD2	2.19	0.43
1:C:102:ASP:OD2	1:C:116:ARG:HB2	2.19	0.43
1:A:351:PRO:HA	1:A:410:ARG:NH1	2.34	0.42
2:B:2:LYS:NZ	2:B:4:GLN:OE1	2.51	0.42
1:E:61:ARG:HB2	1:E:151:ASP:OD2	2.19	0.42
1:G:462:TYR:O	1:G:468:ASN:ND2	2.51	0.42
1:A:33:ASP:CB	1:A:36:ILE:HG13	2.47	0.42
1:A:314:LEU:CD2	1:A:500:ILE:HD11	2.49	0.42
2:B:99:LYS:HD2	2:B:136:LEU:HD11	2.01	0.42
1:E:331:LEU:HD12	1:E:331:LEU:HA	1.87	0.42
1:G:324:LYS:HE2	1:G:429:THR:OG1	2.20	0.42
1:A:62:TYR:CE2	1:A:151:ASP:HB2	2.55	0.42
1:A:252:HIS:HA	1:A:278:ASP:OD2	2.19	0.42
1:A:282:THR:HG21	1:A:287:PHE:HD2	1.85	0.42
2:B:50:ALA:HB3	2:B:53:GLN:HG2	2.01	0.42
2:D:99:LYS:HD2	2:D:136:LEU:HD11	2.00	0.42
1:E:15:VAL:HG11	1:E:238:PHE:CZ	2.54	0.42
1:E:51:LEU:HD22	1:E:72:THR:HG21	2.01	0.42
2:F:86:ARG:CD	2:F:98:LEU:HD22	2.50	0.42
2:H:78:ARG:HA	2:H:124:TYR:HD2	1.84	0.42
1:A:28:GLN:HB2	1:A:417:THR:O	2.20	0.42
1:E:430:ARG:HG3	1:E:492:TRP:NE1	2.35	0.42
1:G:77:VAL:O	1:G:81:ILE:HG13	2.19	0.42
1:A:223:HIS:CD2	1:A:223:HIS:N	2.88	0.42
1:A:306:SER:HA	1:A:307:PRO:HD3	1.93	0.42
1:A:389:LYS:HD2	1:A:408:GLU:HB3	2.02	0.42
2:B:86:ARG:HD2	2:B:98:LEU:HD13	2.02	0.42
1:C:21:ILE:HA	1:C:22:PRO:HD3	1.93	0.42
1:A:230:ARG:HG2	1:A:252:HIS:HB2	2.01	0.42
2:D:97:PHE:CE1	2:D:116:ARG:HG2	2.55	0.42
1:G:196:VAL:HG22	1:G:197:PHE:CD2	2.53	0.42
2:H:88:MSE:HE1	2:H:135:LEU:HD22	2.02	0.42
2:D:70:VAL:HG13	2:D:71:PRO:HD2	2.02	0.42
1:E:68:ASP:OD2	2:F:105:ARG:NH2	2.52	0.42
1:G:173:ASN:ND2	1:G:177:ASP:HB2	2.35	0.42
1:A:27:MSE:HE3	1:A:27:MSE:HB3	1.79	0.42
2:F:92:PRO:HG2	2:F:140:VAL:HA	2.01	0.42
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.81	0.41
2:F:90:SER:HB2	2:F:93:SER:O	2.20	0.41
1:G:112:ILE:HB	1:G:124:VAL:HB	2.01	0.41
1:G:238:PHE:CE2	1:G:239:THR:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:LEU:O	1:E:500:ILE:HG13	2.20	0.41
1:G:8:TRP:NE1	1:G:33:ASP:OD2	2.45	0.41
1:G:240:ASN:O	1:G:244:LEU:HD23	2.20	0.41
1:A:4:PHE:CD2	1:A:232:VAL:HB	2.55	0.41
1:C:31:GLU:CD	1:C:66:ARG:HH11	2.28	0.41
2:H:49:ILE:HD13	2:H:55:ILE:HA	2.02	0.41
2:B:77:LYS:CB	2:B:80:ARG:HD2	2.48	0.41
2:B:98:LEU:HD23	2:B:120:MSE:HE2	2.02	0.41
1:G:18:ARG:HG3	1:G:57:MSE:HG2	2.02	0.41
1:A:45:GLU:OE1	1:A:509:HIS:HB2	2.20	0.41
1:A:98:GLU:HG2	1:A:99:TRP:H	1.86	0.41
2:D:34:ILE:HG13	2:D:44:PHE:HD1	1.86	0.41
1:G:280:VAL:HB	1:G:302:ILE:HG12	2.02	0.41
1:E:39:ILE:HD11	1:E:51:LEU:HD13	2.02	0.41
1:E:426:LEU:HD23	1:E:426:LEU:HA	1.72	0.41
1:C:26:SER:O	1:C:27:MSE:HE3	2.21	0.41
1:C:292:GLN:HG2	1:C:299:ALA:HB1	2.01	0.41
2:D:41:GLN:HE21	2:D:146:HIS:CE1	2.39	0.41
1:G:134:PHE:CD1	1:G:146:LEU:HD11	2.56	0.41
1:G:140:ASP:O	1:G:142:GLN:N	2.54	0.41
2:H:112:ASN:O	2:H:113:HIS:ND1	2.41	0.41
1:A:257:PHE:HB2	1:A:282:THR:HG22	2.02	0.41
2:B:1:MSE:HE2	2:B:1:MSE:HA	2.03	0.41
1:E:64:LEU:HD22	1:E:69:ILE:HG13	2.03	0.41
1:E:360:TYR:CZ	1:E:440:ASN:HB2	2.55	0.41
2:F:11:TRP:CZ2	2:F:56:HIS:ND1	2.89	0.41
2:H:97:PHE:CE1	2:H:116:ARG:HG2	2.55	0.41
1:E:56:TYR:CZ	1:E:58:PRO:HG3	2.56	0.41
1:E:136:LYS:HG3	1:E:146:LEU:HD13	2.02	0.41
1:E:490:LYS:HD3	1:E:490:LYS:HA	1.88	0.41
1:C:306:SER:HA	1:C:307:PRO:HD3	1.94	0.40
1:C:355:LEU:O	1:C:411:PHE:HA	2.22	0.40
2:D:57:GLU:HG3	2:D:134:GLN:HG2	2.02	0.40
2:F:92:PRO:HG3	2:F:141:GLU:H	1.86	0.40
1:G:255:LEU:HD12	1:G:255:LEU:HA	1.83	0.40
1:G:410:ARG:HD3	3:G:613:HOH:O	2.20	0.40
1:A:45:GLU:O	1:A:47:LEU:HG	2.21	0.40
1:C:34:ASP:OD1	1:C:34:ASP:N	2.54	0.40
1:C:168:CYS:HA	1:C:184:LEU:HG	2.02	0.40
1:E:420:LEU:O	1:E:424:GLN:HG3	2.21	0.40
2:H:38:SER:HB3	2:H:41:GLN:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:ARG:C	2:H:107:ASN:N	2.77	0.40
1:C:150:ASP:OD1	1:C:152:ARG:HG3	2.22	0.40
1:G:499:SER:O	1:G:503:ILE:HG13	2.21	0.40
1:C:216:LYS:HA	1:C:216:LYS:HD3	1.76	0.40
1:E:444:GLN:HE21	1:E:456:ASN:ND2	2.19	0.40
1:E:55:ALA:HB3	1:E:57:MSE:HE2	2.04	0.40

All (2) 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)
2:D:48:LEU:N	2:H:46:ASN:O[4_566]	2.05	0.15
2:D:46:ASN:O	2:H:48:LEU:N[4_566]	2.19	0.01

## 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	511/533 (96%)	472 (92%)	37 (7%)	2 (0%)	30	61
1	C	507/533 (95%)	485 (96%)	22 (4%)	0	100	100
1	E	504/533 (95%)	474 (94%)	28 (6%)	2 (0%)	30	61
1	G	504/533 (95%)	463 (92%)	38 (8%)	3 (1%)	21	52
2	B	128/159 (80%)	111 (87%)	15 (12%)	2 (2%)	7	30
2	D	128/159 (80%)	119 (93%)	8 (6%)	1 (1%)	16	47
2	F	128/159 (80%)	118 (92%)	10 (8%)	0	100	100
2	H	128/159 (80%)	115 (90%)	12 (9%)	1 (1%)	16	47
All	All	2538/2768 (92%)	2357 (93%)	170 (7%)	11 (0%)	30	61

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	ILE
1	E	46	ASN
2	H	65	GLN
1	A	46	ASN
2	D	117	SER
1	G	46	ASN
1	G	141	ASP
1	G	296	PRO
1	A	334	LEU
1	E	141	ASP
2	B	34	ILE

### 5.3.2 Protein sidechains [i](#)

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	478/487 (98%)	466 (98%)	12 (2%)	42 69
1	C	474/487 (97%)	455 (96%)	19 (4%)	28 60
1	E	471/487 (97%)	454 (96%)	17 (4%)	31 62
1	G	471/487 (97%)	458 (97%)	13 (3%)	38 66
2	B	126/144 (88%)	120 (95%)	6 (5%)	23 54
2	D	126/144 (88%)	120 (95%)	6 (5%)	23 54
2	F	126/144 (88%)	118 (94%)	8 (6%)	16 45
2	H	126/144 (88%)	119 (94%)	7 (6%)	19 49
All	All	2398/2524 (95%)	2310 (96%)	88 (4%)	30 61

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	MSE
1	A	29	ARG
1	A	54	GLN
1	A	94	ILE
1	A	196	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	314	LEU
1	A	373	LYS
1	A	389	LYS
1	A	396	GLN
1	A	466	LEU
1	A	500	ILE
1	A	511	VAL
2	B	33	THR
2	B	34	ILE
2	B	62	TRP
2	B	76	LEU
2	B	115	GLU
2	B	133	VAL
1	C	1	MSE
1	C	9	SER
1	C	27	MSE
1	C	51	LEU
1	C	57	MSE
1	C	76	SER
1	C	97	LEU
1	C	113	ILE
1	C	170	ASP
1	C	205	GLU
1	C	225	VAL
1	C	269	ASN
1	C	273	ASP
1	C	274	LEU
1	C	316	LYS
1	C	317	SER
1	C	494	GLN
1	C	507	THR
1	C	512	ILE
2	D	62	TRP
2	D	83	SER
2	D	85	THR
2	D	127	GLU
2	D	133	VAL
2	D	154	LEU
1	E	15	VAL
1	E	51	LEU
1	E	54	GLN
1	E	76	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	94	ILE
1	E	113	ILE
1	E	128	VAL
1	E	157	SER
1	E	167	VAL
1	E	210	PRO
1	E	239	THR
1	E	265	SER
1	E	282	THR
1	E	298	GLN
1	E	317	SER
1	E	328	GLN
1	E	480	VAL
2	F	62	TRP
2	F	85	THR
2	F	90	SER
2	F	101	ILE
2	F	113	HIS
2	F	120	MSE
2	F	127	GLU
2	F	133	VAL
1	G	15	VAL
1	G	25	ARG
1	G	27	MSE
1	G	91	VAL
1	G	196	VAL
1	G	267	ILE
1	G	317	SER
1	G	331	LEU
1	G	410	ARG
1	G	467	GLN
1	G	475	ILE
1	G	480	VAL
1	G	512	ILE
2	H	62	TRP
2	H	76	LEU
2	H	88	MSE
2	H	90	SER
2	H	101	ILE
2	H	133	VAL
2	H	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	59	HIS
1	A	82	GLN
1	A	262	ASN
1	A	293	ASN
1	A	303	HIS
1	A	364	GLN
1	A	444	GLN
1	A	456	ASN
1	C	37	HIS
1	C	59	HIS
1	C	82	GLN
1	C	123	HIS
1	C	303	HIS
1	C	456	ASN
2	D	41	GLN
1	E	28	GLN
1	E	46	ASN
1	E	59	HIS
1	E	82	GLN
1	E	93	GLN
1	E	119	GLN
1	E	236	GLN
1	E	292	GLN
1	E	303	HIS
1	E	395	ASN
1	E	415	ASN
1	E	456	ASN
2	F	37	HIS
2	F	65	GLN
2	F	112	ASN
1	G	82	GLN
1	G	224	ASN
1	G	259	HIS
1	G	319	GLN
1	G	350	HIS
1	G	491	ASN
1	G	493	ASN
2	H	56	HIS
2	H	65	GLN
2	H	134	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	511/533 (95%)	0.12	11 (2%) 62 41	1, 24, 70, 88	0
1	C	507/533 (95%)	-0.04	8 (1%) 70 49	1, 15, 63, 103	0
1	E	504/533 (94%)	-0.08	11 (2%) 62 41	1, 16, 62, 100	0
1	G	504/533 (94%)	0.28	25 (4%) 34 18	2, 26, 78, 98	0
2	B	131/159 (82%)	0.62	11 (8%) 17 9	11, 42, 81, 96	0
2	D	131/159 (82%)	0.15	4 (3%) 51 30	3, 23, 55, 67	0
2	F	131/159 (82%)	0.34	8 (6%) 27 15	5, 32, 76, 85	0
2	H	131/159 (82%)	0.40	5 (3%) 44 25	9, 37, 74, 89	0
All	All	2550/2768 (92%)	0.13	83 (3%) 49 29	1, 23, 71, 103	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	66	GLY	5.7
1	G	241	GLN	5.4
1	G	239	THR	5.2
1	E	186	PHE	4.3
1	G	276	TYR	4.1
1	G	238	PHE	4.1
1	G	523	ILE	4.0
2	B	91	TYR	3.8
2	B	139	GLY	3.8
1	G	321	HIS	3.8
2	B	66	GLY	3.6
1	E	523	ILE	3.5
1	G	186	PHE	3.5
1	G	268	GLU	3.4
2	B	12	GLY	3.4
1	A	227	GLU	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	242	GLY	3.4
1	E	28	GLN	3.4
1	G	252	HIS	3.2
1	A	186	PHE	3.1
2	B	32	SER	3.1
1	C	238	PHE	3.1
1	C	186	PHE	3.1
1	C	241	GLN	3.0
1	E	29	ARG	3.0
1	E	321	HIS	3.0
2	F	33	THR	3.0
2	D	69	GLN	2.8
2	F	63	ASN	2.8
2	B	154	LEU	2.8
1	A	245	ASP	2.8
1	A	29	ARG	2.7
1	G	189	SER	2.6
1	A	509	HIS	2.6
1	C	223	HIS	2.6
1	A	189	SER	2.6
2	B	67	ASP	2.6
2	H	32	SER	2.5
2	H	69	GLN	2.5
2	B	39	PRO	2.5
2	H	37	HIS	2.5
2	F	32	SER	2.5
1	C	523	ILE	2.4
2	D	12	GLY	2.4
1	E	241	GLN	2.4
2	F	91	TYR	2.4
2	H	2	LYS	2.4
1	G	295	PHE	2.4
2	D	33	THR	2.4
2	B	37	HIS	2.4
1	E	250	HIS	2.4
1	G	221	ILE	2.3
2	B	94	GLU	2.3
1	A	28	GLN	2.3
2	H	65	GLN	2.3
1	E	227	GLU	2.3
1	C	250	HIS	2.3
1	G	522	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	118	GLY	2.2
1	G	250	HIS	2.2
2	F	64	TYR	2.2
1	E	26	SER	2.2
1	A	238	PHE	2.2
1	A	321	HIS	2.2
1	G	3	TYR	2.2
1	G	267	ILE	2.2
1	A	204	LEU	2.2
2	F	154	LEU	2.1
1	G	240	ASN	2.1
1	E	239	THR	2.1
1	G	294	TYR	2.1
1	G	204	LEU	2.1
1	G	278	ASP	2.1
2	B	146	HIS	2.1
2	F	69	GLN	2.1
1	C	525	GLU	2.1
1	A	226	GLU	2.1
1	G	271	LYS	2.1
1	C	98	GLU	2.1
1	G	237	PRO	2.1
1	E	101	ASP	2.0
2	D	66	GLY	2.0
1	G	509	HIS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.