



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:23 AM GMT

PDB ID : 3AK5
Title : Hemoglobin protease (Hbp) passenger missing domain-2
Authors : Nishimura, K.; Park, S.-Y.; Tame, J.R.H.
Deposited on : 2010-07-07
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

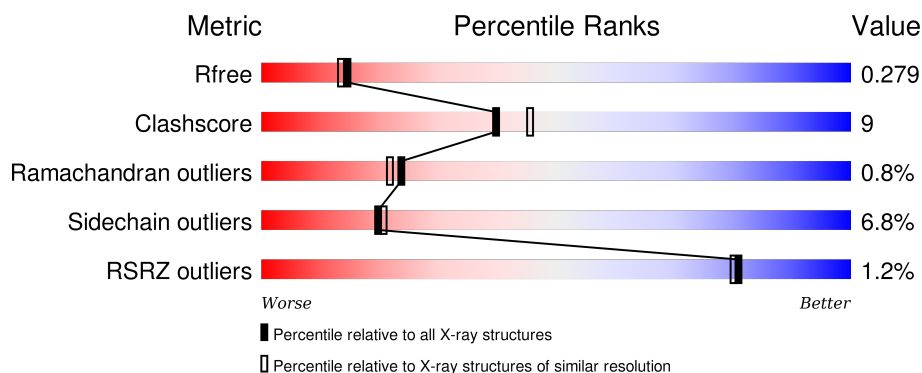
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	975	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	975	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	975	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>
1	D	975	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>..</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30307 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 Hemoglobin-binding protease hbp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	970	Total	C	N	O	S	7	0	0
			7278	4511	1268	1485	14			
1	B	970	Total	C	N	O	S	4	0	0
			7278	4511	1268	1485	14			
1	C	952	Total	C	N	O	S	4	1	0
			7149	4435	1241	1459	14			
1	D	948	Total	C	N	O	S	9	0	0
			7113	4411	1236	1452	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	607	GLY	-	SEE REMARK 999	UNP O88093
B	607	GLY	-	SEE REMARK 999	UNP O88093
C	607	GLY	-	SEE REMARK 999	UNP O88093
D	607	GLY	-	SEE REMARK 999	UNP O88093

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

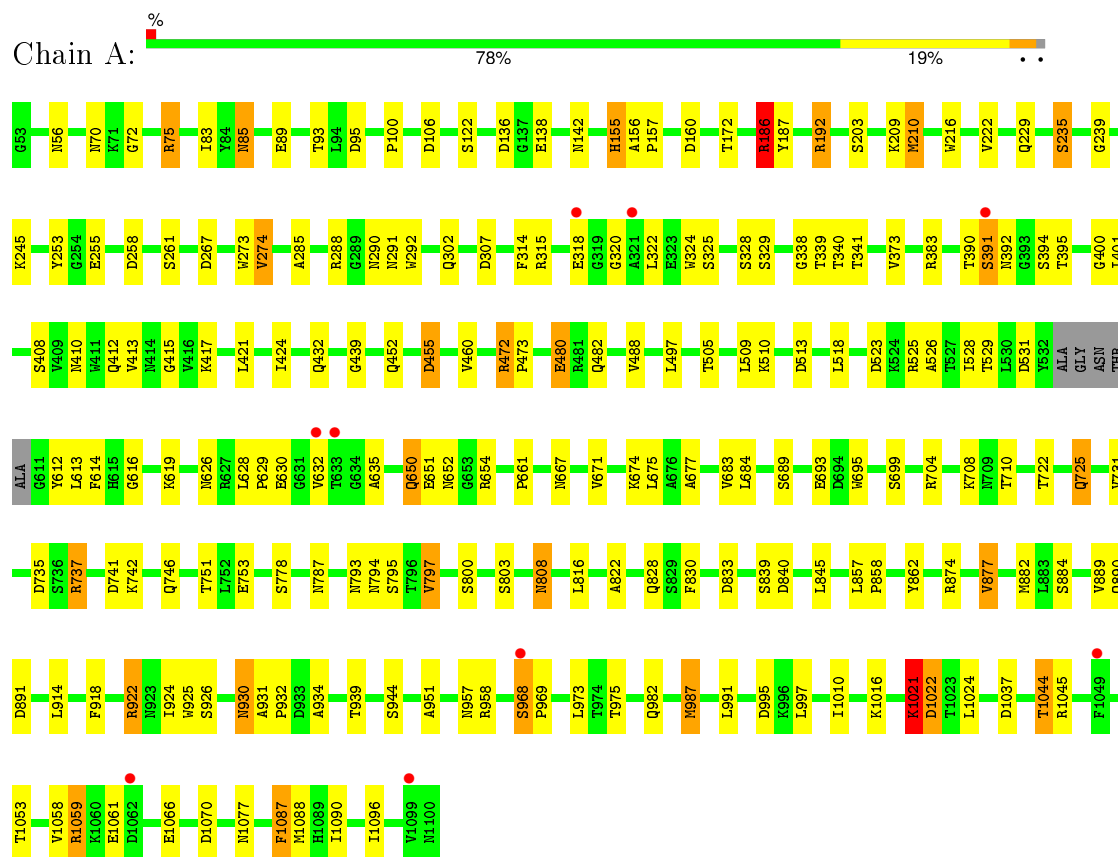
- Molecule 3 is water.

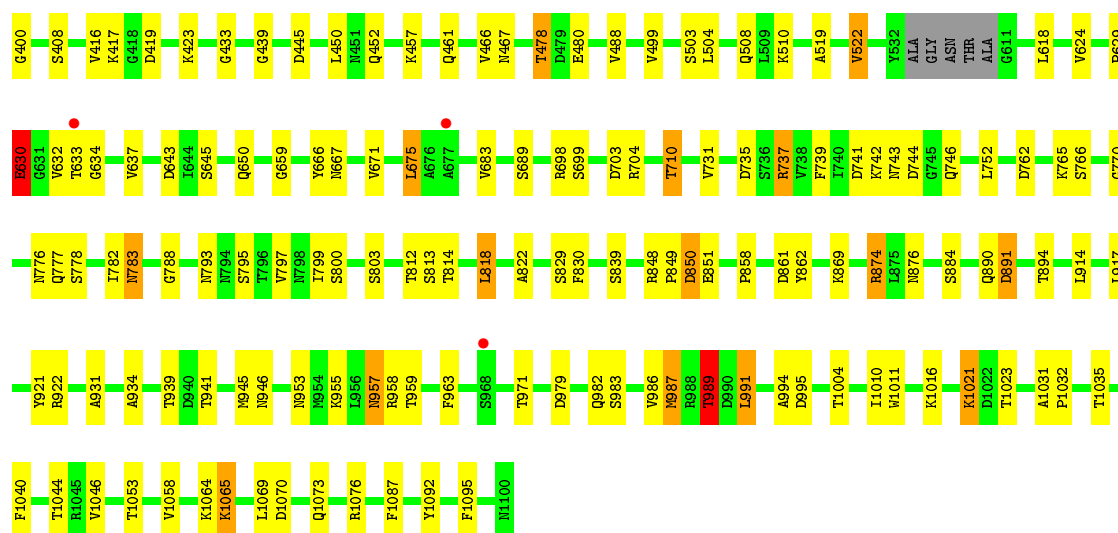
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	426	Total 426	O 426	0	0
3	B	430	Total 430	O 430	0	0
3	C	321	Total 321	O 321	0	0
3	D	308	Total 308	O 308	0	0

3 Residue-property plots

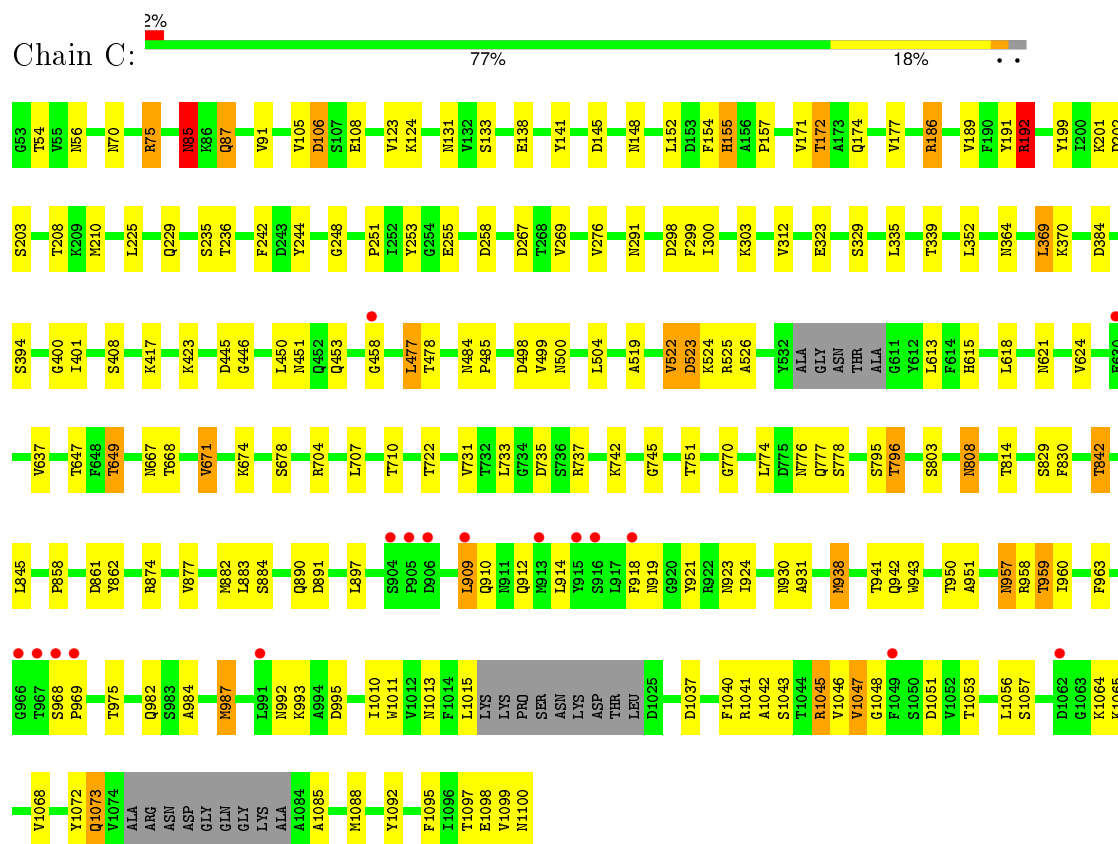
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

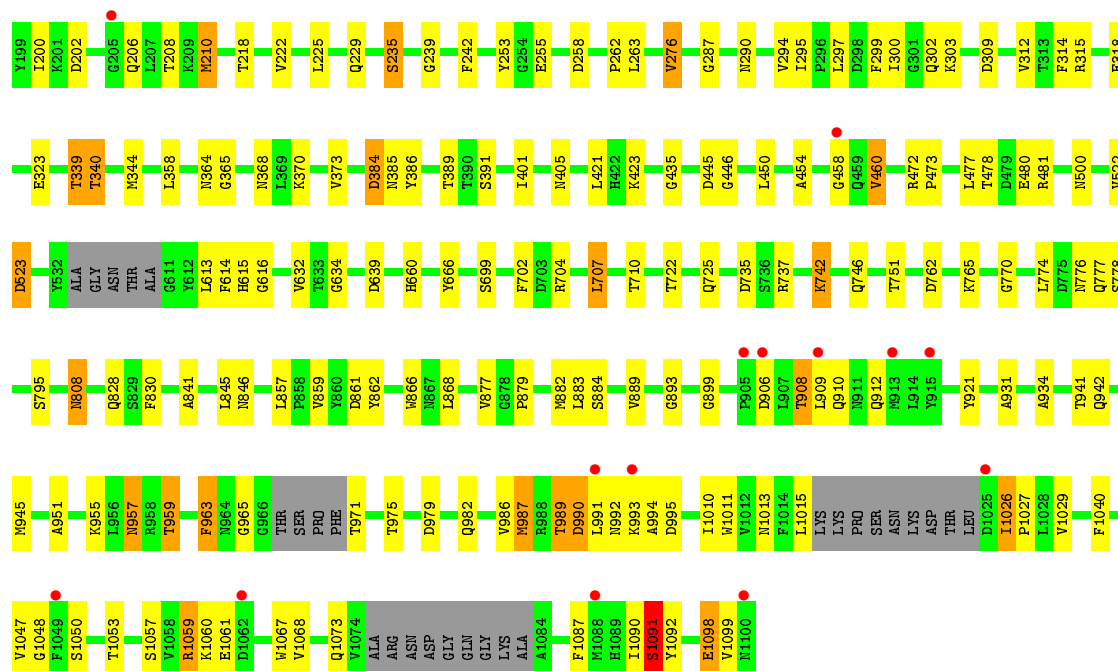
• Molecule 1: Hemoglobin-binding protease hbp





• Molecule 1: Hemoglobin-binding protease hbp





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	292.80 Å 53.94 Å 335.95 Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	48.56 – 2.20 48.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.56-2.20) 93.1 (48.56-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.280 0.224 , 0.279	Depositor DCC
R_{free} test set	11985 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	11 of 239062 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30307	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 94.28 % 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 3.1752e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:
CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	3/7407 (0.0%)	0.99	17/10069 (0.2%)
1	B	1.15	6/7407 (0.1%)	1.04	20/10069 (0.2%)
1	C	1.09	5/7278 (0.1%)	0.99	9/9895 (0.1%)
1	D	1.26	7/7236 (0.1%)	1.12	11/9835 (0.1%)
All	All	1.14	21/29328 (0.1%)	1.04	57/39868 (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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	7

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	89	GLU	CD-OE2	-51.39	0.69	1.25
1	B	851	GLU	CG-CD	-31.69	1.04	1.51
1	B	955	LYS	CE-NZ	29.51	2.22	1.49
1	D	89	GLU	CD-OE1	25.27	1.53	1.25
1	A	619	LYS	CE-NZ	-23.79	0.89	1.49
1	C	138	GLU	CD-OE1	-23.29	1.00	1.25
1	C	138	GLU	CD-OE2	22.94	1.50	1.25
1	A	417	LYS	CE-NZ	-19.25	1.00	1.49
1	C	523	ASP	CG-OD1	18.29	1.67	1.25
1	D	523	ASP	CG-OD2	17.87	1.66	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	523	ASP	CG-OD1	-17.71	0.84	1.25
1	D	138	GLU	CD-OE2	15.79	1.43	1.25
1	D	138	GLU	CD-OE1	-14.74	1.09	1.25
1	C	523	ASP	CG-OD2	-13.01	0.95	1.25
1	A	1021	LYS	CA-CB	-8.54	1.35	1.53
1	D	138	GLU	CG-CD	7.09	1.62	1.51
1	B	144	VAL	CB-CG1	-6.03	1.40	1.52
1	B	302	GLN	CG-CD	5.74	1.64	1.51
1	C	138	GLU	CG-CD	5.67	1.60	1.51
1	B	633	THR	CA-CB	5.45	1.67	1.53
1	B	1070	ASP	CB-CG	-5.01	1.41	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	523	ASP	CB-CG-OD2	-43.35	79.29	118.30
1	D	89	GLU	OE1-CD-OE2	31.72	161.37	123.30
1	C	523	ASP	CB-CG-OD1	-26.34	94.59	118.30
1	D	89	GLU	CG-CD-OE1	-20.08	78.14	118.30
1	B	851	GLU	CG-CD-OE1	19.40	157.10	118.30
1	B	851	GLU	CG-CD-OE2	-18.23	81.85	118.30
1	B	851	GLU	CB-CG-CD	18.09	163.03	114.20
1	A	192	ARG	NE-CZ-NH1	-10.57	115.02	120.30
1	B	192	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	A	192	ARG	NE-CZ-NH2	9.53	125.06	120.30
1	B	192	ARG	NE-CZ-NH2	9.08	124.84	120.30
1	C	192	ARG	NE-CZ-NH2	8.81	124.71	120.30
1	A	186	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	B	307	ASP	CB-CG-OD2	8.69	126.12	118.30
1	C	192	ARG	NE-CZ-NH1	-8.54	116.03	120.30
1	A	136	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	737	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	D	384	ASP	CB-CG-OD1	-7.78	111.30	118.30
1	B	160	ASP	CB-CG-OD2	7.76	125.29	118.30
1	A	186	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	619	LYS	CD-CE-NZ	7.14	128.12	111.70
1	A	267	ASP	CB-CG-OD1	7.02	124.62	118.30
1	C	523	ASP	CB-CG-OD2	6.91	124.52	118.30
1	D	523	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	B	75	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	B	267	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	445	ASP	CB-CG-OD1	6.51	124.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	THR	CB-CA-C	-6.33	94.52	111.60
1	A	922	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	B	737	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	A	307	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	307	ASP	CB-CG-OD1	-6.06	112.85	118.30
1	C	145	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	917	LEU	CA-CB-CG	5.95	128.99	115.30
1	D	318	GLU	CB-CG-CD	-5.78	98.60	114.20
1	A	307	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	818	LEU	CA-CB-CG	5.73	128.47	115.30
1	A	136	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	D	309	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	955	LYS	CD-CE-NZ	-5.60	98.83	111.70
1	B	989	THR	CB-CA-C	-5.54	96.64	111.60
1	A	274	VAL	CG1-CB-CG2	5.54	119.76	110.90
1	C	369	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	C	909	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	874	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	D	132	VAL	CB-CA-C	5.46	121.78	111.40
1	A	513	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	874	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	152	LEU	CB-CG-CD2	-5.39	101.83	111.00
1	C	352	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	472	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	A	455	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	D	182	LEU	CA-CB-CG	5.23	127.33	115.30
1	D	136	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	643	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	737	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	C	75	ARG	NE-CZ-NH1	-5.06	117.77	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	968	SER	Peptide
1	B	1069	LEU	Peptide
1	B	963	PHE	Peptide
1	C	523	ASP	Sidechain
1	C	968	SER	Peptide
1	D	391	SER	Peptide
1	D	523	ASP	Sidechain

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	7278	0	6993	115	0
1	B	7278	0	6993	109	0
1	C	7149	0	6858	141	0
1	D	7113	0	6823	136	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	426	0	0	15	0
3	B	430	0	0	15	0
3	C	321	0	0	9	0
3	D	308	0	0	7	0
All	All	30307	0	27667	497	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 9.

All (497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364[B]:ASN:OD1	1:D:364:ASN:ND2	1.76	1.16
1:B:632:VAL:HG12	1:B:634:GLY:H	1.27	0.99
1:A:401:ILE:HD12	1:A:421:LEU:HD11	1.40	0.99
1:C:842:THR:HG22	3:C:1285:HOH:O	1.62	0.97
1:D:172:THR:HG22	1:D:174:GLN:H	1.31	0.94
1:C:938:MET:HE2	1:C:943:TRP:HB2	1.47	0.94
1:C:1013:ASN:ND2	1:C:1048:GLY:HA3	1.84	0.92
1:C:525:ARG:HE	1:C:621:ASN:HD21	1.18	0.92
1:B:979:ASP:OD1	1:B:1004:THR:HG22	1.69	0.92
1:C:921:TYR:CE2	1:C:942:GLN:NE2	2.37	0.92
1:A:75:ARG:HH21	1:A:75:ARG:HG3	1.32	0.90
1:C:248:GLY:O	1:C:251:PRO:HD3	1.72	0.89
1:A:138:GLU:HG2	3:A:1239:HOH:O	1.71	0.89
1:A:383:ARG:HD3	3:A:1413:HOH:O	1.70	0.89
1:D:1011:TRP:HE3	1:D:1047:VAL:HG23	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:987:MET:HB3	1:D:995:ASP:HB2	1.58	0.86
1:D:85:ASN:ND2	1:D:89:GLU:HG2	1.90	0.86
1:C:921:TYR:HE2	1:C:942:GLN:NE2	1.75	0.84
1:C:450:LEU:O	1:C:478:THR:HG23	1.76	0.84
1:D:1011:TRP:HE3	1:D:1047:VAL:CG2	1.91	0.83
1:A:667:ASN:HB3	1:A:671:VAL:CG2	2.08	0.83
1:C:957:ASN:O	1:C:959:THR:HG22	1.77	0.83
1:B:302:GLN:NE2	3:B:1262:HOH:O	2.14	0.80
1:C:1011:TRP:HE3	1:C:1047:VAL:CG2	1.95	0.80
1:D:1013:ASN:OD1	1:D:1048:GLY:HA3	1.82	0.79
1:C:735:ASP:OD1	1:C:737:ARG:HD3	1.83	0.79
1:D:987:MET:CB	1:D:995:ASP:HB2	2.13	0.78
1:C:647:THR:HG22	1:C:649:THR:HG22	1.65	0.76
1:D:1011:TRP:CE3	1:D:1047:VAL:CG2	2.69	0.76
1:A:401:ILE:CD1	1:A:421:LEU:HD11	2.14	0.76
1:A:735:ASP:OD1	1:A:737:ARG:HD3	1.85	0.76
1:D:192:ARG:NH1	3:D:539:HOH:O	2.19	0.76
1:C:1013:ASN:HD21	1:C:1048:GLY:HA3	1.48	0.75
1:C:649:THR:HG23	3:C:1160:HOH:O	1.86	0.75
1:D:957:ASN:O	1:D:959:THR:HG22	1.86	0.75
1:D:172:THR:HG21	1:D:181:TYR:OH	1.87	0.75
1:C:525:ARG:HE	1:C:621:ASN:ND2	1.83	0.75
1:C:1011:TRP:CE3	1:C:1047:VAL:HG22	2.22	0.74
1:B:225:LEU:HD22	1:B:234:ILE:HG23	1.69	0.74
1:C:192:ARG:NH1	3:C:1153:HOH:O	2.04	0.74
1:D:908:THR:HG22	1:D:909:LEU:H	1.53	0.74
1:B:383:ARG:HD3	3:B:1489:HOH:O	1.87	0.74
1:B:735:ASP:OD1	1:B:737:ARG:HD3	1.88	0.73
1:D:908:THR:HG22	1:D:909:LEU:N	2.04	0.73
1:C:298:ASP:HB2	3:C:1366:HOH:O	1.89	0.72
1:C:186:ARG:HD3	1:C:267:ASP:OD1	1.89	0.72
1:A:987:MET:HB3	1:A:995:ASP:HB2	1.72	0.72
1:C:364[B]:ASN:ND2	1:D:385:ASN:HD22	1.87	0.71
1:C:210:MET:CE	1:C:674:LYS:HB3	2.20	0.71
1:A:987:MET:CB	1:A:995:ASP:HB2	2.21	0.71
1:D:989:THR:HG23	1:D:994:ALA:HB2	1.72	0.71
1:C:938:MET:CE	1:C:943:TRP:HB2	2.21	0.70
1:A:778:SER:O	1:A:795:SER:HB3	1.90	0.70
1:D:196:GLY:HA3	1:D:258:ASP:OD2	1.92	0.70
1:A:72:GLY:O	1:A:75:ARG:NH2	2.26	0.69
1:A:650:GLN:NE2	1:A:652:ASN:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:TRP:HE3	1:C:1047:VAL:HG22	1.54	0.68
1:D:965:GLY:HA3	1:D:971:THR:HG21	1.75	0.68
1:B:503:SER:O	1:B:504:LEU:HD23	1.93	0.68
1:C:154:PHE:HE1	1:C:300:ILE:CD1	2.07	0.67
1:C:210:MET:HA	1:C:210:MET:CE	2.23	0.67
1:A:918:PHE:HA	1:A:924:ILE:HD12	1.76	0.67
1:D:154:PHE:CE1	1:D:300:ILE:HD11	2.29	0.67
1:C:186:ARG:HG2	1:C:269:VAL:HG23	1.76	0.67
1:D:154:PHE:CZ	1:D:300:ILE:HD11	2.29	0.67
1:B:793:ASN:HD22	1:B:812:THR:HB	1.58	0.67
1:C:85:ASN:HB3	1:C:87:GLN:H	1.59	0.67
1:A:1059:ARG:NH1	1:A:1066:GLU:OE1	2.27	0.67
1:C:451:ASN:HD21	1:C:453:GLN:HE21	1.42	0.66
1:C:364[A]:ASN:OD1	1:D:364:ASN:ND2	2.28	0.66
1:C:154:PHE:CE1	1:C:300:ILE:HD11	2.29	0.66
1:B:971:THR:HG22	3:B:1401:HOH:O	1.95	0.66
1:C:210:MET:HE1	1:C:674:LYS:HB3	1.76	0.66
1:B:675:LEU:HD13	1:B:683:VAL:HG21	1.77	0.65
1:B:858:PRO:HB2	1:B:914:LEU:HD23	1.78	0.65
1:B:75:ARG:HG3	1:B:75:ARG:HH21	1.61	0.65
1:A:509:LEU:N	1:A:612:TYR:OH	2.21	0.65
1:B:341:THR:O	3:B:579:HOH:O	2.15	0.65
1:D:198:GLN:NE2	1:D:218:THR:HG23	2.11	0.65
1:D:1011:TRP:CZ2	1:D:1098:GLU:HG2	2.32	0.64
1:D:210:MET:HA	1:D:210:MET:HE2	1.78	0.64
1:B:234:ILE:HG22	1:B:292:TRP:HB2	1.79	0.64
1:A:339:THR:HG23	1:A:340:THR:H	1.61	0.64
1:C:253:TYR:HE2	1:C:255:GLU:OE2	1.81	0.64
1:D:210:MET:CE	1:D:210:MET:HA	2.27	0.64
1:C:731:VAL:HG12	1:C:733:LEU:CD1	2.27	0.64
1:D:323:GLU:HB3	1:D:370:LYS:HD2	1.80	0.64
1:D:229:GLN:HG3	3:D:1326:HOH:O	1.98	0.63
1:D:1013:ASN:ND2	1:D:1015:LEU:HD23	2.13	0.63
1:A:858:PRO:HB2	1:A:914:LEU:HD23	1.81	0.63
1:C:1046:VAL:HG23	3:C:1463:HOH:O	1.97	0.63
1:C:987:MET:HB3	1:C:995:ASP:HB2	1.79	0.63
1:B:667:ASN:HB3	1:B:671:VAL:HG22	1.80	0.62
1:C:91:VAL:HG11	1:C:244:TYR:CE1	2.34	0.62
1:A:973:LEU:HD23	1:A:997:LEU:HD13	1.82	0.62
1:D:1026:ILE:HG22	1:D:1027:PRO:HD2	1.81	0.62
1:B:1058:VAL:CG1	1:B:1065:LYS:HD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLY:HA3	3:B:1130:HOH:O	2.00	0.62
1:D:450:LEU:O	1:D:478:THR:HG23	2.00	0.62
1:C:154:PHE:HE1	1:C:300:ILE:HD11	1.65	0.61
1:A:400:GLY:HA2	3:A:1115:HOH:O	1.99	0.61
1:A:667:ASN:HB3	1:A:671:VAL:HG22	1.82	0.61
1:D:85:ASN:HB2	1:D:89:GLU:H	1.66	0.61
1:C:1072:TYR:O	1:C:1073:GLN:HB3	2.00	0.61
1:C:845:LEU:HD12	1:C:877:VAL:HG22	1.82	0.61
1:B:522:VAL:HG13	3:B:1375:HOH:O	2.00	0.60
1:B:667:ASN:HB3	1:B:671:VAL:CG2	2.32	0.60
1:C:882:MET:HG2	1:C:918:PHE:CZ	2.36	0.60
1:A:186:ARG:HD2	1:A:187:TYR:CZ	2.37	0.60
1:C:154:PHE:CE1	1:C:300:ILE:CD1	2.85	0.59
1:A:918:PHE:HA	1:A:924:ILE:CD1	2.32	0.59
1:D:368:ASN:ND2	3:D:1334:HOH:O	2.35	0.59
1:C:225:LEU:HG	1:C:236:THR:HB	1.84	0.59
1:B:931:ALA:HB1	1:B:934:ALA:HB3	1.85	0.58
1:B:245:LYS:HG3	1:B:246:LEU:N	2.17	0.58
1:D:735:ASP:OD1	1:D:737:ARG:HD3	2.02	0.58
1:C:1011:TRP:CE3	1:C:1047:VAL:CG2	2.81	0.58
1:B:233:MET:O	1:B:234:ILE:HD12	2.02	0.58
1:C:253:TYR:CE2	1:C:255:GLU:OE2	2.56	0.58
1:D:1011:TRP:CE3	1:D:1047:VAL:HG23	2.30	0.58
1:C:1045:ARG:NH1	1:C:1097:THR:OG1	2.34	0.58
1:B:298:ASP:O	1:B:302:GLN:HG3	2.04	0.58
1:A:452:GLN:N	1:A:482:GLN:OE1	2.27	0.58
1:C:1013:ASN:OD1	1:C:1015:LEU:HD23	2.03	0.57
1:C:451:ASN:ND2	1:C:453:GLN:HE21	2.01	0.57
1:D:454:ALA:HA	1:D:460:VAL:HB	1.86	0.57
1:D:85:ASN:HB2	1:D:89:GLU:N	2.19	0.57
1:C:210:MET:HE3	1:C:210:MET:HA	1.87	0.57
1:C:987:MET:CB	1:C:995:ASP:HB2	2.35	0.57
1:B:987:MET:HB3	1:B:995:ASP:HB2	1.86	0.57
1:A:210:MET:CE	1:A:210:MET:HA	2.35	0.57
1:D:778:SER:O	1:D:795:SER:HB3	2.03	0.56
1:D:879:PRO:HG3	1:D:899:GLY:O	2.05	0.56
1:C:707:LEU:HB3	1:C:710:THR:CG2	2.35	0.56
1:A:797:VAL:HG22	1:A:816:LEU:CD1	2.35	0.56
1:A:845:LEU:HD12	1:A:877:VAL:HB	1.87	0.56
1:D:253:TYR:CE2	1:D:255:GLU:OE2	2.58	0.56
1:B:987:MET:CB	1:B:995:ASP:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:GLY:O	1:B:788:GLY:HA3	2.06	0.56
1:C:451:ASN:HD21	1:C:453:GLN:NE2	2.04	0.56
1:B:396:TRP:CH2	1:B:398:GLY:HA3	2.41	0.56
1:A:235:SER:HB2	1:A:291:ASN:HD22	1.70	0.56
1:A:395:THR:CG2	1:A:415:GLY:O	2.54	0.55
1:B:1010:ILE:CD1	1:B:1040:PHE:HB3	2.36	0.55
1:C:1037:ASP:OD1	1:C:1065:LYS:NZ	2.28	0.55
1:B:743:ASN:OD1	1:B:746:GLN:HG3	2.05	0.55
1:A:951:ALA:HB3	1:A:975:THR:HG22	1.89	0.55
1:D:990:ASP:HB3	1:D:992:ASN:H	1.72	0.55
1:A:704:ARG:HD3	1:A:725:GLN:OE1	2.07	0.54
1:C:618:LEU:HD13	1:C:624:VAL:HG21	1.89	0.54
1:B:1058:VAL:HG13	1:B:1065:LYS:HD2	1.88	0.54
1:D:253:TYR:HE2	1:D:255:GLU:OE2	1.91	0.54
1:B:298:ASP:HB2	3:B:1181:HOH:O	2.08	0.54
1:D:154:PHE:CE1	1:D:300:ILE:CD1	2.91	0.54
1:A:186:ARG:HD2	1:A:187:TYR:CE1	2.43	0.54
1:A:958:ARG:HA	1:A:982:GLN:O	2.08	0.54
1:C:862:TYR:CD1	1:C:884:SER:HB3	2.43	0.54
1:D:704:ARG:HD3	1:D:725:GLN:OE1	2.08	0.53
1:C:499:VAL:HG22	1:C:519:ALA:O	2.07	0.53
1:D:845:LEU:HD12	1:D:877:VAL:HG22	1.91	0.53
1:D:1026:ILE:CG2	1:D:1027:PRO:HD2	2.39	0.53
1:D:908:THR:CG2	1:D:909:LEU:H	2.18	0.53
1:D:155:HIS:CD2	1:D:157:PRO:HD3	2.43	0.53
1:D:951:ALA:HB3	1:D:975:THR:HG22	1.89	0.53
1:D:921:TYR:CD2	1:D:942:GLN:HB2	2.44	0.53
1:B:776:ASN:O	1:B:777:GLN:HB2	2.09	0.53
1:C:649:THR:CG2	3:C:1160:HOH:O	2.48	0.53
1:D:861:ASP:O	1:D:883:LEU:HD12	2.08	0.53
1:B:323:GLU:O	1:B:335:LEU:HA	2.09	0.52
1:B:991:LEU:HD22	1:B:1016:LYS:HG3	1.91	0.52
1:A:75:ARG:HH21	1:A:75:ARG:CG	2.11	0.52
1:A:890:GLN:O	1:A:891:ASP:HB2	2.09	0.52
1:D:1010:ILE:CD1	1:D:1040:PHE:HB3	2.39	0.52
1:A:314:PHE:HD2	1:A:322:LEU:HD12	1.74	0.52
1:D:941:THR:H	1:D:959:THR:HB	1.73	0.52
1:B:782:ILE:HD12	1:B:799:ILE:HG12	1.91	0.52
1:C:842:THR:HB	1:C:874:ARG:HB2	1.91	0.52
1:A:626:ASN:HB3	1:A:650:GLN:HG2	1.91	0.52
1:D:987:MET:HB2	1:D:995:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:MET:HB2	1:A:995:ASP:HB2	1.90	0.52
1:B:419:ASP:OD2	3:B:1136:HOH:O	2.19	0.51
1:C:745:GLY:HA2	3:C:1300:HOH:O	2.10	0.51
1:B:186:ARG:HD2	1:B:187:TYR:CZ	2.46	0.51
1:A:674:LYS:O	1:A:677:ALA:HB3	2.10	0.51
1:C:941:THR:H	1:C:959:THR:HB	1.75	0.51
1:A:800:SER:HA	1:A:822:ALA:HB2	1.93	0.51
1:A:930:ASN:ND2	1:A:932:PRO:HD3	2.25	0.51
1:A:395:THR:HG22	1:A:415:GLY:O	2.10	0.51
1:B:632:VAL:HG12	1:B:634:GLY:N	2.11	0.51
1:C:1013:ASN:ND2	1:C:1048:GLY:CA	2.67	0.51
1:C:707:LEU:HB3	1:C:710:THR:HG22	1.91	0.51
1:D:1059:ARG:HG2	1:D:1060:LYS:N	2.25	0.51
1:D:423:LYS:C	1:D:423:LYS:HD3	2.32	0.51
1:B:186:ARG:HG3	1:B:269:VAL:HG23	1.94	0.50
1:A:83:ILE:HA	3:A:1490:HOH:O	2.11	0.50
1:A:930:ASN:C	1:A:930:ASN:HD22	2.13	0.50
1:D:1090:ILE:HG22	1:D:1091:SER:O	2.11	0.50
1:B:302:GLN:HG2	3:B:1376:HOH:O	2.10	0.50
1:A:488:VAL:HG11	1:A:497:LEU:HD22	1.92	0.50
1:C:229:GLN:HG2	1:C:229:GLN:O	2.11	0.50
1:A:1010:ILE:HD12	1:A:1010:ILE:N	2.26	0.50
1:A:235:SER:CB	1:A:291:ASN:HD22	2.24	0.50
1:B:958:ARG:HA	1:B:982:GLN:O	2.11	0.50
1:A:210:MET:HE3	1:A:210:MET:HA	1.94	0.50
1:A:797:VAL:HG22	1:A:816:LEU:HD12	1.93	0.50
1:C:722:THR:O	1:C:770:GLY:HA3	2.11	0.50
1:C:613:LEU:HD21	1:C:615:HIS:CE1	2.45	0.50
1:B:255:GLU:OE1	1:B:285:ALA:HA	2.12	0.50
1:B:800:SER:HA	1:B:822:ALA:HB2	1.93	0.50
1:C:795:SER:C	1:C:814:THR:HG23	2.33	0.49
1:D:931:ALA:HB1	1:D:934:ALA:HB3	1.94	0.49
1:C:408:SER:OG	3:C:1224:HOH:O	2.19	0.49
1:B:450:LEU:O	1:B:478:THR:HG23	2.12	0.49
1:D:632:VAL:HG12	1:D:634:GLY:H	1.77	0.49
1:C:776:ASN:O	1:C:777:GLN:HB2	2.12	0.49
1:B:56:ASN:C	1:B:56:ASN:OD1	2.51	0.49
1:B:314:PHE:O	3:B:1458:HOH:O	2.20	0.49
1:D:990:ASP:O	1:D:991:LEU:HB2	2.13	0.49
1:A:693:GLU:HG2	3:A:1455:HOH:O	2.12	0.49
1:C:323:GLU:HB3	1:C:370:LYS:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1013:ASN:ND2	1:D:1015:LEU:CD2	2.76	0.49
1:C:861:ASP:O	1:C:883:LEU:HD12	2.12	0.49
1:D:921:TYR:CD1	1:D:1092:TYR:HD2	2.30	0.49
1:C:91:VAL:CG1	1:C:244:TYR:CD1	2.96	0.49
1:D:722:THR:O	1:D:770:GLY:HA3	2.12	0.49
1:C:921:TYR:CD1	1:C:1092:TYR:HD2	2.31	0.49
1:B:452:GLN:HG2	1:B:461:GLN:C	2.34	0.49
1:C:918:PHE:HA	1:C:924:ILE:CD1	2.42	0.48
1:A:613:LEU:HD21	1:A:741:ASP:HB2	1.95	0.48
1:A:742:LYS:HE3	1:A:753:GLU:OE2	2.13	0.48
1:C:667:ASN:HB3	1:C:671:VAL:HG22	1.94	0.48
1:A:324:TRP:CE2	1:A:373:VAL:HG21	2.48	0.48
1:C:774:LEU:HB3	1:C:778:SER:HB2	1.94	0.48
1:D:122:SER:OG	1:D:123:VAL:N	2.46	0.48
1:C:938:MET:HE2	1:C:943:TRP:CB	2.32	0.48
1:D:992:ASN:O	1:D:1026:ILE:HD13	2.13	0.48
1:A:472:ARG:N	1:A:473:PRO:CD	2.77	0.48
1:B:72:GLY:O	1:B:75:ARG:NH2	2.47	0.48
1:C:303:LYS:HE2	1:C:303:LYS:HA	1.94	0.48
1:C:951:ALA:HB3	1:C:975:THR:HG22	1.96	0.48
1:D:868:LEU:HB3	3:D:1306:HOH:O	2.13	0.48
1:C:522:VAL:HG13	1:C:524:LYS:H	1.78	0.48
1:D:472:ARG:N	1:D:473:PRO:CD	2.76	0.48
1:C:731:VAL:HG12	1:C:733:LEU:HD13	1.95	0.48
1:A:412:GLN:O	3:A:1274:HOH:O	2.20	0.48
1:C:1013:ASN:HD22	1:C:1048:GLY:HA3	1.71	0.48
1:D:1010:ILE:HD11	1:D:1040:PHE:HB3	1.96	0.48
1:B:186:ARG:HD2	1:B:187:TYR:CE1	2.49	0.48
1:A:156:ALA:N	1:A:157:PRO:HD3	2.29	0.48
1:A:518:LEU:HD21	1:A:528:ILE:HD12	1.96	0.48
1:D:762:ASP:OD2	1:D:765:LYS:HE3	2.14	0.48
1:D:445:ASP:OD1	1:D:446:GLY:N	2.44	0.48
1:D:1053:THR:HB	1:D:1073:GLN:HB2	1.95	0.48
1:B:989:THR:HG23	1:B:994:ALA:HB2	1.96	0.47
1:A:1021:LYS:O	1:A:1022:ASP:HB2	2.12	0.47
1:C:423:LYS:HD3	1:C:423:LYS:C	2.33	0.47
1:C:1046:VAL:HG12	1:C:1047:VAL:N	2.28	0.47
1:A:629:PRO:O	1:A:632:VAL:HG13	2.13	0.47
1:B:650:GLN:HG2	1:B:710:THR:HG21	1.95	0.47
1:C:1010:ILE:CD1	1:C:1040:PHE:HB3	2.44	0.47
1:A:290:ASN:HB2	1:A:292:TRP:CH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:LYS:HB2	1:A:751:THR:HB	1.97	0.47
1:B:659:GLY:HA2	1:B:698:ARG:HG2	1.96	0.47
1:B:1021:LYS:HE3	1:B:1021:LYS:HA	1.96	0.47
1:D:299:PHE:O	1:D:302:GLN:HB2	2.14	0.47
1:A:1087:PHE:HA	1:A:1090:ILE:HG13	1.96	0.47
1:D:458:GLY:O	1:D:481:ARG:NH1	2.45	0.47
1:A:505:THR:HA	1:A:529:THR:O	2.14	0.47
1:A:862:TYR:CD1	1:A:884:SER:HB3	2.49	0.47
1:D:154:PHE:HE1	1:D:300:ILE:CD1	2.27	0.47
1:A:930:ASN:ND2	1:A:930:ASN:C	2.68	0.47
1:A:939:THR:HA	1:A:957:ASN:O	2.15	0.47
1:C:229:GLN:CG	1:C:229:GLN:O	2.62	0.47
3:A:1409:HOH:O	1:B:138:GLU:HG2	2.15	0.47
1:B:849:PRO:HG3	1:B:876:ASN:ND2	2.30	0.47
1:D:614:PHE:CZ	1:D:616:GLY:HA3	2.50	0.47
1:D:908:THR:CG2	1:D:909:LEU:N	2.71	0.47
1:D:239:GLY:HA3	1:D:287:GLY:O	2.15	0.47
1:A:793:ASN:OD1	1:A:794:ASN:ND2	2.48	0.47
1:D:172:THR:HG22	1:D:173:ALA:N	2.30	0.46
1:D:989:THR:HG22	1:D:993:LYS:O	2.14	0.46
1:D:989:THR:CG2	1:D:994:ALA:HB2	2.43	0.46
1:D:846:ASN:ND2	1:D:859:VAL:HG22	2.29	0.46
1:B:637:VAL:HG11	1:B:739:PHE:HB2	1.97	0.46
1:A:931:ALA:HB1	1:A:934:ALA:HB3	1.97	0.46
1:C:1011:TRP:CZ2	1:C:1098:GLU:HG3	2.50	0.46
1:D:368:ASN:HA	1:D:389:THR:O	2.15	0.46
1:A:922:ARG:HB2	3:A:1452:HOH:O	2.15	0.46
1:B:400:GLY:HA2	3:B:1104:HOH:O	2.14	0.46
1:B:423:LYS:HD3	1:B:423:LYS:C	2.36	0.46
1:B:630:GLU:HG2	1:B:630:GLU:H	1.40	0.46
1:A:889:VAL:HG11	1:A:934:ALA:HB2	1.98	0.46
1:D:963:PHE:CD1	1:D:963:PHE:N	2.84	0.46
1:D:963:PHE:HB2	1:D:995:ASP:OD2	2.15	0.46
1:A:1077:ASN:HB2	3:A:1172:HOH:O	2.15	0.46
1:C:54:THR:OG1	1:C:199:TYR:HB2	2.16	0.46
1:A:75:ARG:NH2	1:A:75:ARG:HG3	2.15	0.46
1:A:85:ASN:HB3	1:A:89:GLU:H	1.81	0.46
1:C:731:VAL:HG12	1:C:733:LEU:HD11	1.98	0.46
1:D:294:VAL:O	1:D:295:ILE:C	2.55	0.46
1:A:412:GLN:HG2	1:A:432:GLN:HB3	1.97	0.45
1:A:628:LEU:HD13	1:A:632:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:958:ARG:HA	1:C:982:GLN:O	2.16	0.45
1:D:339:THR:HG22	1:D:340:THR:HG22	1.98	0.45
1:B:433:GLY:N	1:B:452:GLN:OE1	2.50	0.45
1:B:202:ASP:OD1	1:B:206:GLN:HB3	2.17	0.45
1:B:1035:THR:O	1:B:1065:LYS:HE2	2.16	0.45
1:A:651:GLU:HG3	1:A:708:LYS:HB3	1.97	0.45
1:B:390:THR:OG1	1:B:394:SER:HB2	2.16	0.45
1:D:85:ASN:CB	1:D:89:GLU:H	2.29	0.45
1:D:1057:SER:O	1:D:1068:VAL:HG12	2.17	0.45
1:C:105:VAL:O	1:C:106:ASP:C	2.53	0.45
1:C:525:ARG:HG3	1:C:526:ALA:N	2.31	0.45
1:C:858:PRO:HB2	1:C:914:LEU:HD23	1.98	0.45
1:C:85:ASN:HB3	1:C:87:GLN:N	2.29	0.45
1:D:666:TYR:HA	3:D:1300:HOH:O	2.17	0.45
1:C:445:ASP:OD1	1:C:446:GLY:N	2.47	0.45
1:D:435:GLY:HA3	3:D:1295:HOH:O	2.16	0.45
1:C:707:LEU:HD22	1:C:710:THR:HG21	1.99	0.45
1:A:383:ARG:NH1	3:A:1105:HOH:O	2.50	0.44
1:C:796:THR:N	1:C:814:THR:HG23	2.31	0.44
1:D:477:LEU:O	1:D:500:ASN:HB3	2.17	0.44
1:C:1098:GLU:C	1:C:1100:ASN:H	2.21	0.44
1:D:989:THR:O	1:D:1015:LEU:HB2	2.18	0.44
1:D:862:TYR:CD1	1:D:884:SER:HB3	2.53	0.44
1:B:75:ARG:NH2	1:B:75:ARG:HG3	2.31	0.44
1:C:877:VAL:HG21	1:C:883:LEU:HD22	1.99	0.44
1:C:1013:ASN:HD22	1:C:1047:VAL:C	2.20	0.44
1:B:939:THR:HA	1:B:957:ASN:O	2.17	0.44
1:D:96:LYS:HA	1:D:96:LYS:HD3	1.70	0.44
1:C:897:LEU:HD22	1:C:938:MET:HE3	1.99	0.44
1:D:941:THR:HB	1:D:959:THR:HB	2.00	0.44
1:A:1024:LEU:O	1:A:1070:ASP:HA	2.18	0.44
1:D:172:THR:CG2	1:D:175:GLY:H	2.29	0.44
1:C:963:PHE:HB2	1:C:995:ASP:OD2	2.18	0.44
1:D:1059:ARG:HD3	1:D:1061:GLU:HB2	2.00	0.44
1:D:235:SER:HB2	1:D:290:ASN:O	2.17	0.44
1:A:1096:ILE:HD12	1:A:1096:ILE:HA	1.75	0.44
1:A:1044:THR:HG22	1:A:1045:ARG:HG3	1.99	0.44
1:C:201:LYS:O	1:C:242:PHE:CZ	2.70	0.44
1:C:154:PHE:CZ	1:C:300:ILE:HD11	2.52	0.44
1:B:783:ASN:ND2	3:B:1389:HOH:O	2.45	0.44
1:C:795:SER:C	1:C:796:THR:OG1	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:VAL:HG22	1:B:519:ALA:O	2.17	0.44
1:B:466:VAL:HG12	1:B:467:ASN:N	2.31	0.44
1:D:196:GLY:O	1:D:198:GLN:HG2	2.18	0.44
1:D:989:THR:HB	1:D:991:LEU:H	1.82	0.44
1:D:120:ILE:O	1:D:156:ALA:HA	2.17	0.44
1:C:477:LEU:O	1:C:500:ASN:HB3	2.18	0.44
1:A:951:ALA:O	1:A:975:THR:HA	2.18	0.43
1:B:795:SER:O	1:B:814:THR:HA	2.18	0.43
1:D:120:ILE:HG13	1:D:157:PRO:HD2	1.99	0.43
1:D:1087:PHE:HA	1:D:1090:ILE:HG13	1.99	0.43
1:C:174:GLN:O	1:C:177:VAL:HG23	2.18	0.43
1:C:960:ILE:HG13	1:C:984:ALA:HB3	1.98	0.43
1:C:931:ALA:H	1:C:950:THR:HG23	1.83	0.43
1:D:774:LEU:HD22	1:D:778:SER:HB3	2.00	0.43
1:B:741:ASP:HB3	1:B:744:ASP:HB2	2.00	0.43
1:C:830:PHE:CD2	1:C:830:PHE:C	2.91	0.43
1:C:498:ASP:OD1	1:C:498:ASP:C	2.56	0.43
1:D:299:PHE:CE2	1:D:303:LYS:HE3	2.54	0.43
1:A:1037:ASP:OD1	1:A:1058:VAL:HG11	2.19	0.43
1:C:668:THR:OG1	1:C:671:VAL:HG13	2.19	0.43
1:A:142:ASN:ND2	1:A:160:ASP:OD1	2.41	0.43
1:B:1010:ILE:HD11	1:B:1040:PHE:CD2	2.54	0.43
1:A:122:SER:HB3	1:A:155:HIS:NE2	2.33	0.43
1:C:1010:ILE:HD12	1:C:1010:ILE:N	2.34	0.43
1:C:1041:ARG:HD2	1:C:1042:ALA:O	2.18	0.43
1:D:69:GLU:HB3	1:D:71:LYS:HD2	1.99	0.43
1:C:192:ARG:HH22	1:C:258:ASP:CG	2.21	0.43
1:D:56:ASN:HB2	1:D:242:PHE:CE1	2.54	0.43
1:D:125:HIS:ND1	1:D:153:ASP:OD2	2.44	0.43
1:C:1043:SER:O	1:C:1053:THR:HG23	2.19	0.43
1:D:263:LEU:HD23	1:D:276:VAL:HG22	2.01	0.43
1:D:1098:GLU:C	1:D:1098:GLU:CD	2.78	0.43
1:B:931:ALA:HB1	1:B:934:ALA:CB	2.47	0.43
1:C:1056:LEU:HA	1:C:1068:VAL:O	2.19	0.43
1:A:100:PRO:HB3	1:A:273:TRP:CD1	2.54	0.43
1:B:192:ARG:HD2	3:B:1101:HOH:O	2.19	0.43
1:B:762:ASP:HA	1:B:765:LYS:HD2	2.01	0.43
1:B:830:PHE:O	1:B:861:ASP:HA	2.19	0.43
1:D:1026:ILE:O	1:D:1068:VAL:HA	2.18	0.43
1:D:955:LYS:HG3	1:D:979:ASP:HB3	2.01	0.43
1:D:1029:VAL:HB	1:D:1067:TRP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLN:HG2	1:A:229:GLN:O	2.19	0.43
1:B:629:PRO:O	1:B:632:VAL:CG2	2.67	0.42
1:A:704:ARG:HE	1:A:704:ARG:HB2	1.75	0.42
1:B:778:SER:O	1:B:795:SER:HB3	2.19	0.42
1:D:986:VAL:HG22	1:D:1011:TRP:HB2	2.00	0.42
1:B:324:TRP:CE2	1:B:335:LEU:HD11	2.52	0.42
1:D:105:VAL:HG22	1:D:262:PRO:HG3	2.01	0.42
1:A:614:PHE:CZ	1:A:616:GLY:HA3	2.54	0.42
1:D:808:ASN:HD22	1:D:828:GLN:HB3	1.83	0.42
1:C:484:ASN:HA	1:C:485:PRO:HD3	1.90	0.42
1:A:302:GLN:NE2	3:A:1262:HOH:O	2.49	0.42
1:A:56:ASN:C	1:A:56:ASN:OD1	2.58	0.42
1:B:862:TYR:CD1	1:B:884:SER:HB3	2.55	0.42
1:C:923:ASN:O	1:C:924:ILE:HG13	2.19	0.42
1:B:957:ASN:ND2	1:B:958:ARG:HG3	2.34	0.42
1:C:1057:SER:O	1:C:1068:VAL:HG12	2.19	0.42
1:B:783:ASN:ND2	1:B:800:SER:OG	2.53	0.42
1:D:889:VAL:HG11	1:D:934:ALA:HB2	2.01	0.42
1:A:944:SER:HB2	1:A:1088:MET:HE3	2.00	0.42
1:B:618:LEU:HD13	1:B:624:VAL:HG21	2.01	0.42
1:D:344:MET:HG3	1:D:358:LEU:HD11	2.01	0.42
1:D:314:PHE:CD1	1:D:365:GLY:HA2	2.55	0.42
1:A:329:SER:HA	3:A:1233:HOH:O	2.18	0.42
1:A:155:HIS:CD2	1:A:157:PRO:HD3	2.55	0.42
1:C:960:ILE:HD12	1:C:1095:PHE:CD2	2.55	0.42
1:B:105:VAL:O	1:B:106:ASP:C	2.54	0.42
1:A:258:ASP:O	1:A:261:SER:HB3	2.19	0.42
1:B:890:GLN:O	1:B:891:ASP:HB2	2.19	0.42
1:C:155:HIS:CD2	1:C:157:PRO:HD3	2.54	0.42
1:A:689:SER:HB2	3:A:1218:HOH:O	2.19	0.42
1:A:925:TRP:CD1	1:A:926:SER:N	2.88	0.42
1:C:171:VAL:O	1:C:172:THR:C	2.56	0.42
1:B:196:GLY:O	1:B:197:THR:C	2.58	0.42
1:A:455:ASP:OD1	1:A:455:ASP:C	2.58	0.42
1:A:216:TRP:CZ3	1:A:671:VAL:HG11	2.54	0.42
1:A:480:GLU:HG2	3:A:1426:HOH:O	2.20	0.42
1:D:613:LEU:HD21	1:D:615:HIS:CE1	2.54	0.42
1:C:369:LEU:HD23	1:C:394:SER:HB3	2.02	0.42
1:D:182:LEU:CD1	1:D:225:LEU:O	2.68	0.42
1:B:261:SER:HB2	1:B:262:PRO:HD2	2.02	0.42
1:A:635:ALA:HA	1:A:654:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:PRO:HA	1:A:695:TRP:HA	2.02	0.42
1:B:396:TRP:CZ2	1:B:398:GLY:HA3	2.55	0.42
1:B:116:ASN:HB3	1:B:119:TYR:HB2	2.02	0.42
1:D:198:GLN:HE22	1:D:218:THR:HG23	1.82	0.41
1:B:416:VAL:O	1:B:417:LYS:C	2.57	0.41
1:D:83:ILE:HG13	1:D:91:VAL:HG22	2.02	0.41
1:C:613:LEU:HD12	1:C:637:VAL:O	2.19	0.41
1:C:930:ASN:HA	1:C:950:THR:HG22	2.02	0.41
1:C:931:ALA:H	1:C:950:THR:CG2	2.32	0.41
1:D:776:ASN:O	1:D:777:GLN:HB2	2.20	0.41
1:C:401:ILE:HG21	1:C:401:ILE:HD13	1.86	0.41
1:C:918:PHE:HA	1:C:924:ILE:HD11	2.02	0.41
1:B:743:ASN:O	1:B:746:GLN:HG2	2.19	0.41
1:D:401:ILE:HD12	1:D:421:LEU:HD11	2.02	0.41
1:A:288:ARG:HD2	3:A:1459:HOH:O	2.20	0.41
1:B:1031:ALA:O	1:B:1032:PRO:C	2.56	0.41
1:C:1013:ASN:OD1	1:C:1015:LEU:CD2	2.67	0.41
1:D:841:ALA:C	3:D:1213:HOH:O	2.58	0.41
1:D:202:ASP:OD1	1:D:206:GLN:HB3	2.21	0.41
1:C:890:GLN:O	1:C:891:ASP:HB2	2.21	0.41
1:A:675:LEU:HD13	1:A:683:VAL:HG21	2.03	0.41
1:C:108:GLU:HG2	1:C:133:SER:HB2	2.03	0.41
1:B:986:VAL:HG22	1:B:1011:TRP:HB2	2.02	0.41
1:C:131:ASN:HA	1:C:141:TYR:O	2.21	0.41
1:A:390:THR:CG2	1:A:394:SER:H	2.34	0.41
1:D:742:LYS:HB2	1:D:751:THR:HB	2.02	0.41
1:A:340:THR:CG2	1:A:341:THR:N	2.84	0.41
1:C:1010:ILE:HD11	1:C:1040:PHE:HB3	2.02	0.41
1:A:390:THR:OG1	1:A:413:VAL:HG22	2.21	0.41
1:B:848:ARG:C	1:B:850:ASP:H	2.23	0.41
1:A:391:SER:HB2	1:B:508:GLN:HE22	1.86	0.41
1:B:457:LYS:HG2	3:B:1408:HOH:O	2.21	0.41
1:A:830:PHE:C	1:A:830:PHE:CD2	2.93	0.41
1:B:666:TYR:OH	1:B:746:GLN:NE2	2.54	0.41
1:A:390:THR:HG21	1:A:394:SER:N	2.35	0.41
1:A:93:THR:HG23	1:A:95:ASP:OD2	2.20	0.41
1:B:645:SER:O	1:B:703:ASP:HB2	2.21	0.41
1:A:808:ASN:HD22	1:A:828:GLN:HB3	1.85	0.41
1:B:85:ASN:HB3	1:B:89:GLU:H	1.86	0.41
1:D:1013:ASN:HD21	1:D:1015:LEU:HD23	1.85	0.41
1:B:1035:THR:O	1:B:1065:LYS:CE	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:877:VAL:HG21	1:D:883:LEU:HD22	2.03	0.41
1:D:344:MET:HE3	1:D:373:VAL:HG13	2.03	0.41
1:A:255:GLU:OE1	1:A:285:ALA:HA	2.20	0.41
1:D:639:ASP:O	1:D:660:HIS:HB2	2.20	0.41
1:B:752:LEU:HD23	1:B:752:LEU:HA	1.93	0.41
1:A:930:ASN:HD22	1:A:932:PRO:HD3	1.85	0.40
1:B:874:ARG:HD3	1:B:894:THR:HB	2.02	0.40
1:B:921:TYR:CD1	1:B:1092:TYR:HD2	2.40	0.40
1:D:707:LEU:HD22	1:D:710:THR:HG21	2.02	0.40
1:D:830:PHE:C	1:D:830:PHE:CD2	2.95	0.40
1:B:161:LYS:NZ	1:B:398:GLY:O	2.40	0.40
1:C:299:PHE:O	1:C:303:LYS:HG2	2.22	0.40
1:B:457:LYS:HB2	1:B:457:LYS:HE3	1.63	0.40
1:A:525:ARG:CG	1:A:526:ALA:N	2.84	0.40
1:B:322:LEU:HD23	1:B:337:GLN:HB3	2.03	0.40
1:C:808:ASN:ND2	1:C:829:SER:H	2.19	0.40
1:D:945:MET:HE3	1:D:945:MET:HB2	1.94	0.40
1:A:833:ASP:C	1:A:833:ASP:OD2	2.60	0.40
1:D:866:TRP:CE2	1:D:883:LEU:HD11	2.55	0.40
1:D:143:ILE:HG23	1:D:157:PRO:HB3	2.04	0.40
1:C:148:ASN:HA	1:C:155:HIS:HB3	2.03	0.40
1:B:99:MET:SD	1:B:100:PRO:HD2	2.60	0.40
1:A:239:GLY:HA2	1:A:253:TYR:HB2	2.03	0.40
1:B:941:THR:O	1:B:959:THR:HG23	2.21	0.40
1:C:189:VAL:CG2	1:C:191:TYR:CE1	3.05	0.40
1:C:124:LYS:HE2	1:C:152:LEU:O	2.22	0.40
1:B:922:ARG:HB2	3:B:1475:HOH:O	2.22	0.40
1:C:742:LYS:HB2	1:C:751:THR:HB	2.03	0.40
1:B:959:THR:O	1:B:983:SER:HB3	2.21	0.40
1:C:400:GLY:HA2	3:C:1:HOH:O	2.20	0.40
1:C:56:ASN:OD1	1:C:56:ASN:C	2.60	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	966/975 (99%)	898 (93%)	55 (6%)	13 (1%)	15	11
1	B	966/975 (99%)	900 (93%)	61 (6%)	5 (0%)	34	35
1	C	945/975 (97%)	876 (93%)	63 (7%)	6 (1%)	30	29
1	D	938/975 (96%)	870 (93%)	60 (6%)	8 (1%)	21	19
All	All	3815/3900 (98%)	3544 (93%)	239 (6%)	32 (1%)	24	22

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	GLY
1	A	1022	ASP
1	C	85	ASN
1	D	85	ASN
1	A	85	ASN
1	A	320	GLY
1	A	531	ASP
1	B	203	SER
1	B	318	GLU
1	C	1073	GLN
1	C	1085	ALA
1	A	318	GLU
1	A	510	LYS
1	A	840	ASP
1	A	969	PRO
1	A	1061	GLU
1	B	630	GLU
1	B	891	ASP
1	D	908	THR
1	B	85	ASN
1	D	982	GLN
1	D	1050	SER
1	D	1091	SER
1	D	460	VAL
1	A	328	SER
1	C	1099	VAL
1	A	439	GLY
1	D	1099	VAL
1	A	424	ILE
1	C	969	PRO

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Mol	Chain	Res	Type
1	D	893	GLY
1	C	458	GLY

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	785/787 (100%)	735 (94%)	50 (6%)	22	24
1	B	785/787 (100%)	721 (92%)	64 (8%)	14	13
1	C	772/787 (98%)	724 (94%)	48 (6%)	23	25
1	D	767/787 (98%)	719 (94%)	48 (6%)	22	24
All	All	3109/3148 (99%)	2899 (93%)	210 (7%)	20	21

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	75	ARG
1	A	106	ASP
1	A	155	HIS
1	A	172	THR
1	A	186	ARG
1	A	192	ARG
1	A	203	SER
1	A	209	LYS
1	A	210	MET
1	A	222	VAL
1	A	235	SER
1	A	245	LYS
1	A	274	VAL
1	A	315	ARG
1	A	325	SER
1	A	391	SER
1	A	392	ASN
1	A	408	SER

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Mol	Chain	Res	Type
1	A	410	ASN
1	A	460	VAL
1	A	480	GLU
1	A	523	ASP
1	A	630	GLU
1	A	650	GLN
1	A	684	LEU
1	A	699	SER
1	A	710	THR
1	A	722	THR
1	A	725	GLN
1	A	731	VAL
1	A	746	GLN
1	A	787	ASN
1	A	797	VAL
1	A	803	SER
1	A	808	ASN
1	A	839	SER
1	A	857	LEU
1	A	877	VAL
1	A	882	MET
1	A	930	ASN
1	A	968	SER
1	A	987	MET
1	A	991	LEU
1	A	1016	LYS
1	A	1021	LYS
1	A	1044	THR
1	A	1053	THR
1	A	1059	ARG
1	A	1087	PHE
1	B	70	ASN
1	B	83	ILE
1	B	91	VAL
1	B	106	ASP
1	B	151	SER
1	B	155	HIS
1	B	186	ARG
1	B	192	ARG
1	B	203	SER
1	B	222	VAL
1	B	234	ILE

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Mol	Chain	Res	Type
1	B	259	SER
1	B	274	VAL
1	B	276	VAL
1	B	302	GLN
1	B	318	GLU
1	B	337	GLN
1	B	339	THR
1	B	341	THR
1	B	352	LEU
1	B	391	SER
1	B	392	ASN
1	B	408	SER
1	B	478	THR
1	B	480	GLU
1	B	488	VAL
1	B	510	LYS
1	B	522	VAL
1	B	630	GLU
1	B	675	LEU
1	B	689	SER
1	B	699	SER
1	B	704	ARG
1	B	710	THR
1	B	731	VAL
1	B	742	LYS
1	B	766	SER
1	B	783	ASN
1	B	797	VAL
1	B	803	SER
1	B	813	SER
1	B	818	LEU
1	B	829	SER
1	B	839	SER
1	B	850	ASP
1	B	869	LYS
1	B	945	MET
1	B	946	ASN
1	B	953	ASN
1	B	957	ASN
1	B	987	MET
1	B	989	THR
1	B	991	LEU

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Mol	Chain	Res	Type
1	B	1021	LYS
1	B	1023	THR
1	B	1044	THR
1	B	1046	VAL
1	B	1053	THR
1	B	1064	LYS
1	B	1065	LYS
1	B	1073	GLN
1	B	1076	ARG
1	B	1087	PHE
1	B	1095	PHE
1	C	70	ASN
1	C	75	ARG
1	C	85	ASN
1	C	87	GLN
1	C	106	ASP
1	C	123	VAL
1	C	155	HIS
1	C	172	THR
1	C	186	ARG
1	C	192	ARG
1	C	202	ASP
1	C	203	SER
1	C	208	THR
1	C	235	SER
1	C	276	VAL
1	C	291	ASN
1	C	312	VAL
1	C	329	SER
1	C	335	LEU
1	C	339	THR
1	C	384	ASP
1	C	417	LYS
1	C	477	LEU
1	C	504	LEU
1	C	522	VAL
1	C	649	THR
1	C	671	VAL
1	C	678	SER
1	C	704	ARG
1	C	796	THR
1	C	803	SER

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Mol	Chain	Res	Type
1	C	808	ASN
1	C	842	THR
1	C	909	LEU
1	C	910	GLN
1	C	912	GLN
1	C	919	ASN
1	C	938	MET
1	C	957	ASN
1	C	959	THR
1	C	987	MET
1	C	992	ASN
1	C	993	LYS
1	C	1045	ARG
1	C	1047	VAL
1	C	1051	ASP
1	C	1064	LYS
1	C	1088	MET
1	D	70	ASN
1	D	75	ARG
1	D	83	ILE
1	D	89	GLU
1	D	106	ASP
1	D	132	VAL
1	D	144	VAL
1	D	155	HIS
1	D	182	LEU
1	D	184	LYS
1	D	192	ARG
1	D	200	ILE
1	D	208	THR
1	D	210	MET
1	D	222	VAL
1	D	235	SER
1	D	276	VAL
1	D	297	LEU
1	D	312	VAL
1	D	315	ARG
1	D	339	THR
1	D	340	THR
1	D	384	ASP
1	D	386	TYR
1	D	405	ASN

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Mol	Chain	Res	Type
1	D	480	GLU
1	D	522	VAL
1	D	699	SER
1	D	702	PHE
1	D	707	LEU
1	D	742	LYS
1	D	746	GLN
1	D	808	ASN
1	D	857	LEU
1	D	882	MET
1	D	906	ASP
1	D	910	GLN
1	D	912	GLN
1	D	957	ASN
1	D	959	THR
1	D	963	PHE
1	D	987	MET
1	D	989	THR
1	D	990	ASP
1	D	1026	ILE
1	D	1059	ARG
1	D	1091	SER
1	D	1098	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	174	GLN
1	A	271	ASN
1	A	291	ASN
1	A	302	GLN
1	A	410	ASN
1	A	432	GLN
1	A	451	ASN
1	A	808	ASN
1	A	912	GLN
1	A	930	ASN
1	A	946	ASN
1	A	964	ASN
1	A	1100	ASN
1	B	87	GLN

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Mol	Chain	Res	Type
1	B	174	GLN
1	B	432	GLN
1	B	451	ASN
1	B	746	GLN
1	B	783	ASN
1	B	793	ASN
1	B	957	ASN
1	B	1020	ASN
1	C	85	ASN
1	C	174	GLN
1	C	350	ASN
1	C	432	GLN
1	C	451	ASN
1	C	467	ASN
1	C	621	ASN
1	C	725	GLN
1	C	794	ASN
1	C	808	ASN
1	C	912	GLN
1	C	919	ASN
1	C	946	ASN
1	C	957	ASN
1	C	964	ASN
1	C	992	ASN
1	C	1000	ASN
1	D	85	ASN
1	D	174	GLN
1	D	350	ASN
1	D	368	ASN
1	D	385	ASN
1	D	392	ASN
1	D	405	ASN
1	D	743	ASN
1	D	808	ASN
1	D	957	ASN
1	D	992	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	970/975 (99%)	-0.21	9 (0%) 85 85	13, 31, 53, 66	4 (0%)
1	B	970/975 (99%)	-0.19	5 (0%) 91 91	13, 30, 53, 70	2 (0%)
1	C	952/975 (97%)	-0.18	17 (1%) 71 70	14, 32, 54, 69	2 (0%)
1	D	948/975 (97%)	-0.18	14 (1%) 76 75	15, 32, 54, 65	4 (0%)
All	All	3840/3900 (98%)	-0.19	45 (1%) 81 80	13, 31, 54, 70	12 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	991	LEU	6.1
1	D	1049	PHE	5.5
1	B	633	THR	5.2
1	C	968	SER	5.2
1	D	909	LEU	5.0
1	C	1049	PHE	4.6
1	D	991	LEU	4.5
1	C	966	GLY	4.5
1	C	909	LEU	4.4
1	D	1088	MET	4.1
1	C	967	THR	3.9
1	A	632	VAL	3.6
1	B	321	ALA	3.6
1	D	913	MET	3.5
1	D	906	ASP	3.3
1	C	913	MET	3.1
1	A	968	SER	3.0
1	C	906	ASP	2.9
1	B	677	ALA	2.9
1	C	969	PRO	2.8
1	D	1062	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	458	GLY	2.8
1	C	915	TYR	2.7
1	C	904	SER	2.6
1	A	633	THR	2.6
1	B	968	SER	2.5
1	C	1062	ASP	2.5
1	D	915	TYR	2.5
1	D	458	GLY	2.4
1	D	905	PRO	2.4
1	D	993	LYS	2.4
1	D	1025	ASP	2.4
1	A	318	GLU	2.4
1	C	905	PRO	2.4
1	A	391	SER	2.4
1	D	205	GLY	2.3
1	D	1100	ASN	2.3
1	A	321	ALA	2.3
1	B	104	ALA	2.2
1	A	1049	PHE	2.2
1	C	916	SER	2.2
1	C	918	PHE	2.2
1	A	1062	ASP	2.1
1	A	1099	VAL	2.0
1	C	630	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	1200	1/1	0.99	0.13	0.96	22,22,22,22	0
2	CA	C	1200	1/1	1.00	0.10	0.08	19,19,19,19	0
2	CA	B	1200	1/1	0.99	0.10	-0.34	19,19,19,19	0
2	CA	D	1200	1/1	0.99	0.10	-1.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.