Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:16 PM GMT

PDB ID	:	1EVU
Title	:	HUMAN FACTOR XIII WITH CALCIUM BOUND IN THE ION SITE
Authors	:	Garzon, R.J.; Pratt, K.P.; Bishop, P.D.; Le Trong, I.; Stenkamp, R.E.; Teller, D.C.
Deposited on	:	2000-04-20
Resolution	:	2.01 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

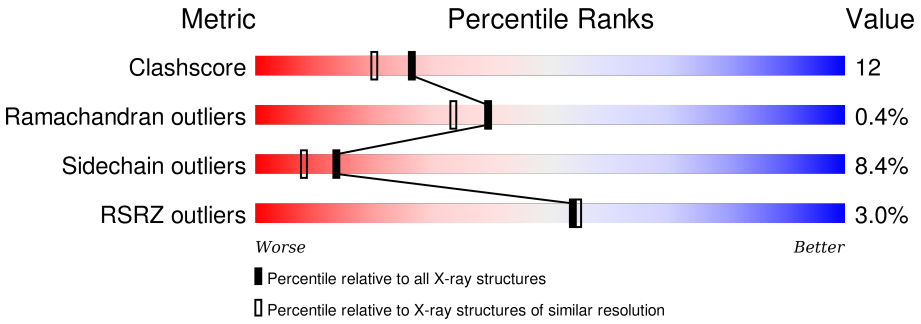
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	731	4% 62% 28% 5% • •
1	B	731	2% 69% 23% 5% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SAC	A	1	-	-	X	-
3	PGO	B	1203	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12593 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 COAGULATION FACTOR XIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	3	0
			5709	3618	981	1084	26			
1	B	708	Total	C	N	O	S	0	4	0
			5718	3623	988	1081	26			

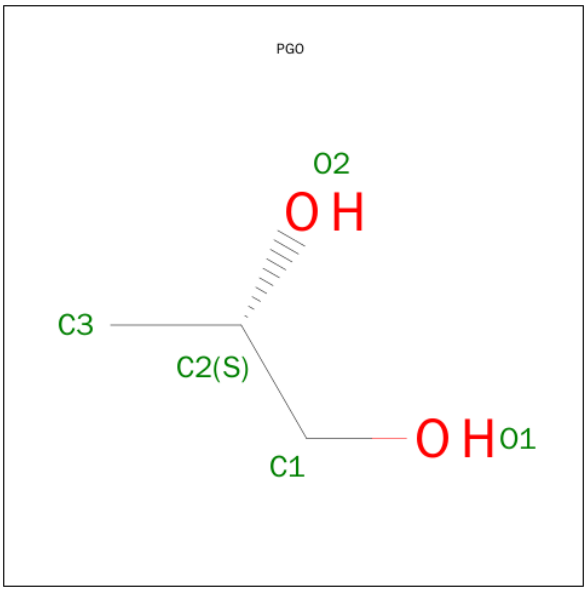
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SAC	SER	MODIFIED RESIDUE	UNP P00488
B	1	SAC	SER	MODIFIED RESIDUE	UNP P00488

- 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		

- Molecule 3 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is water.

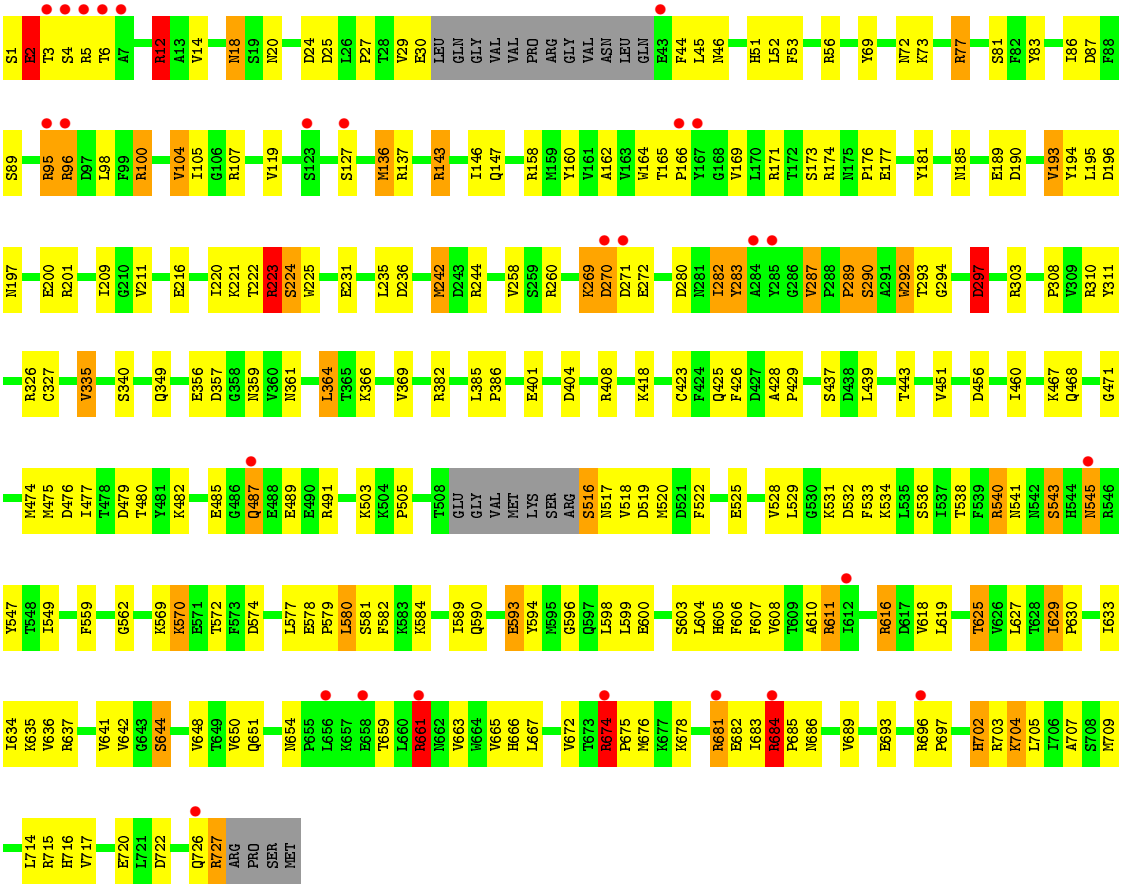
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	542	Total	O	0	0
			542	542		
4	B	617	Total	O	0	0
			617	617		

3 Residue-property plots (i)

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.

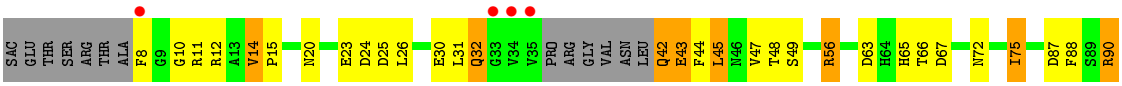
- Molecule 1: COAGULATION FACTOR XIII

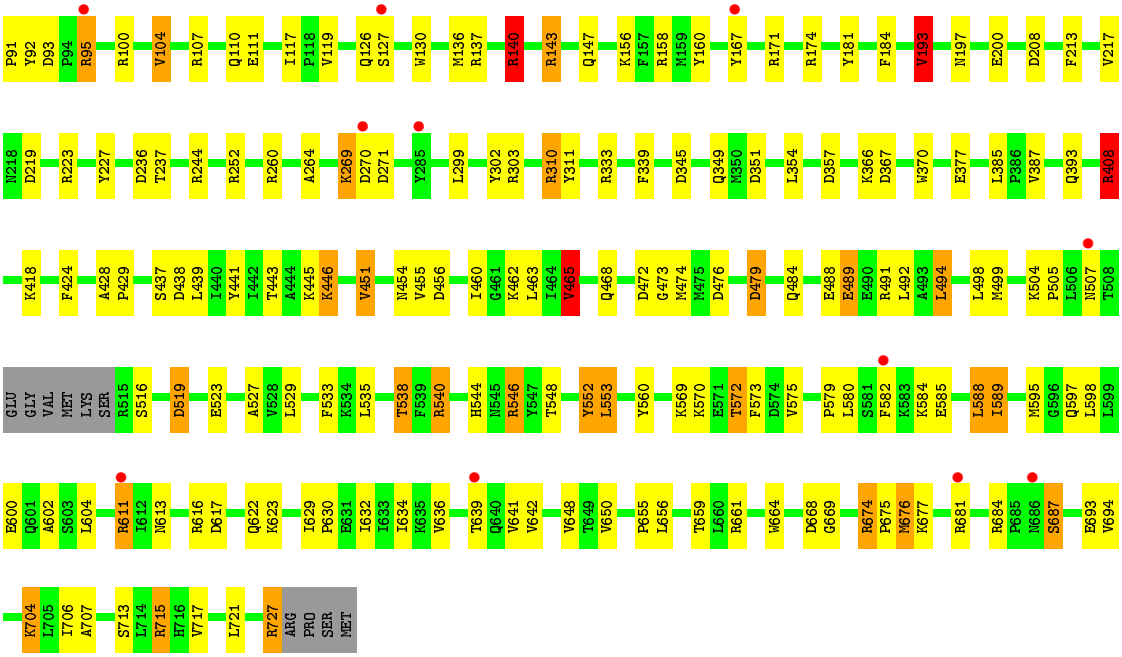
Chain A:



- Molecule 1: COAGULATION FACTOR XIII

Chain B:




P91 Y92 D93 P94 R95 R100 V104 R107 Q110 E111 I117 P118 V119 Q126 S127 W130 M136 R137 R140 R143 Q147 K156 F157 R158 N159 Y160 Y167 R171 R174 Y181 F184 V193 N197 E200 D208 F213 V217
N218 D219 R223 Y227 D236 T237 R244 R252 R260 A264 K269 D270 D271 Y285 L299 Y302 R303 R310 Y311 R333 F339 D345 Q349 N350 D351 L354 D357 K366 D367 W370 E377 L385 F386 V387 Q393 R408
K418 F424 A428 P429 S437 D438 L439 I440 Y441 I442 T443 A444 K445 K446 V451 N454 V455 D456 I460 G461 K462 L463 I464 V465 Q468 D472 G473 M474 M475 D476 D479 Q484 E488 E489 E490 R491 L492 A493 L494 L498 M499 K504 P505 L506 N507 T508
GLU GLY VAL MET LYS SER R515 S516 D519 E523 A527 V528 L529 F533 K534 L535 T538 F539 R540 H544 N545 R546 Y547 T548 Y552 L553 Y560 K569 K570 E571 T572 F573 D574 V575 P579 L580 S581 F582 K583 K584 E585 I588 I589 M595 G596 Q597 L598 L599
E600 Q601 A602 S603 L604 R611 I612 M613 R616 D617 Q622 K623 I629 P630 E631 I632 I633 I634 K635 V636 T639 Q640 V641 V642 V648 T649 V650 P655 L656 T659 L660 R661 W664 D668 G669 R674 P675 M676 K677 R681 R684 P685 N686 S687 E693 V694
K704 L705 I706 A707 S713 L714 R715 H716 V717 L721 R727 ARG PRO SER MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.17Å 70.76Å 133.82Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	20.66 – 2.01 20.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.66-2.01) 91.6 (20.66-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.266 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 111498 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12593	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SAC, PGO, 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	0.66	0/5834	1.47	71/7916 (0.9%)
1	B	0.72	0/5851	1.58	81/7938 (1.0%)
All	All	0.69	0/11685	1.53	152/15854 (1.0%)

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	5
1	B	0	3
All	All	0	8

There are no bond length outliers.

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	ARG	NE-CZ-NH2	-25.62	107.49	120.30
1	A	100	ARG	CD-NE-CZ	13.58	142.62	123.60
1	B	260	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	A	137	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	B	351	ASP	CB-CG-OD1	11.38	128.54	118.30
1	A	158	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	A	223	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	A	223	ARG	NE-CZ-NH2	-10.65	114.98	120.30
1	A	357	ASP	CB-CG-OD2	10.51	127.76	118.30
1	B	441	TYR	CB-CG-CD1	-10.48	114.71	121.00
1	B	611	ARG	NE-CZ-NH1	-10.47	115.07	120.30
1	A	143	ARG	NE-CZ-NH2	-10.23	115.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	244	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	B	441	TYR	CB-CG-CD2	9.88	126.93	121.00
1	B	727	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	B	11	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	56	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	107	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	B	11	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	B	107	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	A	77	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	A	100	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	303	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	B	333	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	B	715	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	B	56	ARG	NH1-CZ-NH2	8.40	128.64	119.40
1	A	171	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	A	190	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	326	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	B	143	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	B	681	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	B	674	ARG	NE-CZ-NH2	8.19	124.39	120.30
1	B	140	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	193	VAL	CA-CB-CG1	8.02	122.94	110.90
1	B	479	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	171	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	B	107	ARG	CD-NE-CZ	7.86	134.60	123.60
1	B	727	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	171	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	A	540	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	87	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	611	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	B	219	ASP	CB-CG-OD1	7.49	125.04	118.30
1	B	408	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	B	23	GLU	OE1-CD-OE2	-7.32	114.52	123.30
1	B	310[A]	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	B	310[B]	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	B	252	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	B	588	LEU	CA-CB-CG	7.21	131.88	115.30
1	A	532	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	408	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	703	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	A	244	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	83	TYR	CB-CG-CD2	-7.14	116.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	552	TYR	CB-CG-CD1	-7.11	116.73	121.00
1	B	56	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	B	476	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	171	ARG	CD-NE-CZ	7.04	133.46	123.60
1	A	69	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	A	476	ASP	CB-CG-OD1	6.96	124.56	118.30
1	B	367	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	593	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	A	104	VAL	CA-CB-CG2	6.79	121.08	110.90
1	B	140	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	616	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	174	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	158	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	137	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	401	GLU	CG-CD-OE1	6.68	131.66	118.30
1	A	260	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	201	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	674	ARG	CD-NE-CZ	6.63	132.88	123.60
1	B	465	VAL	CG1-CB-CG2	6.61	121.47	110.90
1	B	302	TYR	CB-CG-CD1	-6.46	117.12	121.00
1	A	158	ARG	CD-NE-CZ	6.44	132.62	123.60
1	A	242	MET	CG-SD-CE	6.41	110.46	100.20
1	A	479	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	24	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	594	TYR	CB-CG-CD2	6.36	124.82	121.00
1	A	221	LYS	CA-CB-CG	6.35	127.37	113.40
1	A	143	ARG	CD-NE-CZ	6.35	132.49	123.60
1	A	684	ARG	CD-NE-CZ	6.32	132.44	123.60
1	B	357	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	727	ARG	CD-NE-CZ	6.30	132.43	123.60
1	B	30	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	B	588	LEU	CB-CG-CD2	6.25	121.63	111.00
1	B	260	ARG	NH1-CZ-NH2	6.20	126.22	119.40
1	A	382	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	335	VAL	CA-CB-CG1	6.13	120.09	110.90
1	B	236	ASP	CB-CG-OD1	6.13	123.81	118.30
1	B	668	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	532	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	499	MET	CA-CB-CG	6.03	123.55	113.30
1	B	227	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	B	87	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	208	ASP	CB-CG-OD2	-6.01	112.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	270	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	357	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	560	TYR	CB-CG-CD1	5.90	124.54	121.00
1	B	92	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	158	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	222	THR	N-CA-CB	5.81	121.35	110.30
1	A	143	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	104	VAL	CA-CB-CG2	5.76	119.55	110.90
1	B	95	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	622	GLN	CA-CB-CG	5.75	126.05	113.40
1	A	83	TYR	CB-CG-CD1	5.73	124.44	121.00
1	B	345	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	326	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	A	283	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	B	63	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	600	GLU	C-N-CA	5.66	135.86	121.70
1	B	111	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	B	438	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	607	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	A	77	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	223	ARG	CD-NE-CZ	-5.55	115.83	123.60
1	B	681	ARG	CD-NE-CZ	5.55	131.37	123.60
1	A	401	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	B	107	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
1	B	160	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	B	140	ARG	O-C-N	-5.49	113.91	122.70
1	A	661	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	297	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	69	TYR	CB-CG-CD1	5.41	124.25	121.00
1	B	387	VAL	CA-CB-CG1	5.41	119.02	110.90
1	A	216	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	B	208	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	30	GLU	N-CA-CB	5.39	120.31	110.60
1	B	333	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	174	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	A	283	TYR	CB-CG-CD1	5.36	124.22	121.00
1	A	193	VAL	CA-CB-CG1	5.31	118.86	110.90
1	A	236	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	637	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	479	ASP	OD1-CG-OD2	-5.27	113.28	123.30
1	A	674	ARG	CG-CD-NE	5.25	122.82	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	404	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	611	ARG	CG-CD-NE	5.20	122.73	111.80
1	A	605	HIS	CA-CB-CG	-5.20	104.76	113.60
1	A	303	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	107	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	423	CYS	O-C-N	-5.12	114.50	122.70
1	B	302	TYR	O-C-N	-5.12	114.50	122.70
1	B	90	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	489	GLU	CA-CB-CG	5.10	124.62	113.40
1	B	333	ARG	CD-NE-CZ	-5.09	116.47	123.60
1	A	160	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	147	GLN	OE1-CD-NE2	5.08	133.58	121.90
1	A	25	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	594	TYR	CB-CG-CD1	-5.05	117.97	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ILE	Mainchain
1	A	12[B]	ARG	Mainchain
1	A	2	GLU	Peptide
1	A	3	THR	Peptide
1	A	596	GLY	Peptide
1	B	32	GLN	Peptide
1	B	632	ILE	Mainchain
1	B	75	ILE	Mainchain

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	5709	0	5546	171	0
1	B	5718	0	5564	116	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	5	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	542	0	0	11	0
4	B	617	0	0	18	0
All	All	12593	0	11118	276	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 12.

All (276) 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:629:ILE:HD11	1:A:717:VAL:HG22	1.27	1.08
1:B:548:THR:HG22	1:B:613:ASN:HD22	1.15	1.07
1:B:44:PHE:O	1:B:45:LEU:HB2	1.53	1.06
1:A:528:VAL:HB	1:A:531:LYS:HD3	1.43	1.00
1:B:12[A]:ARG:HD3	4:B:1759:HOH:O	1.62	0.99
1:B:630:PRO:HG3	1:B:655:PRO:HG3	1.51	0.93
1:B:443:THR:HB	1:B:451:VAL:HG13	1.49	0.92
1:A:290:SER:HG	1:A:716:HIS:HD1	0.90	0.90
1:A:242:MET:CE	1:A:258:VAL:HG22	2.09	0.82
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.61	0.81
1:B:595:MET:HA	1:B:595:MET:HE2	1.63	0.80
1:A:681:ARG:HH11	1:A:681:ARG:HB3	1.45	0.80
1:A:559[B]:PHE:CD1	1:B:8:PHE:HE2	1.97	0.80
1:A:528:VAL:HB	1:A:531:LYS:CD	2.11	0.80
1:A:95:ARG:NH1	1:A:96:ARG:NH1	2.31	0.79
1:A:559[A]:PHE:CE1	1:A:599:LEU:HD13	2.20	0.76
1:A:641:VAL:HB	1:A:644:SER:HB2	1.66	0.75
1:B:519:ASP:HB3	1:B:540:ARG:HD3	1.69	0.75
1:B:629:ILE:HG23	1:B:630:PRO:HD2	1.68	0.75
1:A:681:ARG:HD2	1:A:682:GLU:HG2	1.69	0.74
1:A:684:ARG:H	1:A:684:ARG:HD2	1.53	0.73
1:A:633:ILE:HB	1:A:651:GLN:HB3	1.71	0.72
1:A:335:VAL:HG22	1:A:477:ILE:HD11	1.70	0.72
1:B:595:MET:HA	1:B:595:MET:CE	2.21	0.71
1:A:290:SER:OG	1:A:716:HIS:ND1	2.09	0.71
1:A:242:MET:HE2	1:A:258:VAL:HG22	1.74	0.70
1:B:529:LEU:HD21	1:B:656:LEU:HD21	1.75	0.69
1:A:559[A]:PHE:CD1	1:A:599:LEU:HD13	2.28	0.68
1:A:5:ARG:O	1:A:6:THR:HB	1.93	0.68
1:A:100:ARG:HG2	1:A:164:TRP:CZ3	2.28	0.68
1:B:548:THR:HG22	1:B:613:ASN:ND2	2.00	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ARG:HG3	1:B:582:PHE:CE2	2.30	0.67
1:B:197:ASN:ND2	1:B:200:GLU:OE1	2.25	0.66
1:A:418:LYS:HD2	1:A:480:THR:O	1.96	0.66
1:B:569:LYS:CD	1:B:589:ILE:HD13	2.26	0.65
1:A:272:GLU:O	4:A:1507:HOH:O	2.14	0.64
1:A:650:VAL:HG11	1:A:665:VAL:HG11	1.80	0.64
1:A:642:VAL:HG23	1:A:726:GLN:O	1.97	0.64
1:A:727:ARG:HA	1:A:727:ARG:HH11	1.62	0.64
1:A:1:SAC:C	1:A:1:SAC:H2A1	2.25	0.63
1:B:349:GLN:OE1	1:B:505:PRO:HD2	1.99	0.63
1:B:156:LYS:HD2	1:B:181:TYR:CZ	2.33	0.62
1:A:726:GLN:O	1:A:727:ARG:HB2	1.99	0.62
1:A:1:SAC:HB2	1:B:713:SER:O	1.99	0.62
1:A:46:ASN:HD22	1:A:89:SER:HB3	1.64	0.62
1:A:242:MET:HE1	1:A:258:VAL:HG13	1.82	0.62
1:A:676:MET:CE	1:A:693:GLU:HG2	2.29	0.62
1:B:472:ASP:OD2	1:B:704:LYS:NZ	2.33	0.61
1:B:674:ARG:HD2	1:B:675:PRO:HD2	1.82	0.61
1:A:2:GLU:OE1	1:B:598:LEU:HD12	1.99	0.61
1:A:100:ARG:HB2	1:A:119:VAL:O	2.02	0.60
1:A:559[B]:PHE:HD1	1:A:599:LEU:HD13	1.66	0.60
1:A:570:LYS:N	1:A:570:LYS:HD2	2.17	0.60
1:A:629:ILE:HD12	1:A:630:PRO:HD2	1.82	0.60
1:A:18:ASN:C	1:A:18:ASN:HD22	2.05	0.60
4:A:1583:HOH:O	1:B:366:LYS:HE3	2.00	0.60
1:A:629:ILE:CD1	1:A:717:VAL:HG22	2.18	0.60
1:B:694:VAL:HG12	4:B:1525:HOH:O	2.01	0.60
1:B:544:HIS:CE1	1:B:580:LEU:HD11	2.37	0.59
1:A:439:LEU:HB2	1:A:456:ASP:HB3	1.85	0.59
1:A:269:LYS:O	1:A:270:ASP:HB2	2.03	0.59
1:A:468:GLN:HG3	1:A:471:GLY:H	1.67	0.59
1:A:51:HIS:HB3	4:A:1391:HOH:O	2.02	0.59
1:B:269:LYS:HD2	4:B:1257:HOH:O	2.01	0.59
1:A:672:VAL:O	4:A:1332:HOH:O	2.17	0.59
1:B:569:LYS:HD3	1:B:589:ILE:HD13	1.84	0.58
1:B:629:ILE:CG2	1:B:630:PRO:HD2	2.33	0.58
1:A:629:ILE:HD12	1:A:630:PRO:CD	2.34	0.58
1:B:538:THR:HG21	1:B:584:LYS:NZ	2.18	0.58
1:A:629:ILE:HD11	1:A:717:VAL:CG2	2.18	0.58
1:A:709:MET:HE3	1:A:717:VAL:HG21	1.85	0.58
1:A:224:SER:HB2	1:A:720:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:OE1	1:B:595:MET:HE1	2.05	0.57
1:A:516:SER:O	1:A:517:ASN:HB2	2.03	0.57
1:A:225:TRP:CE2	1:A:294:GLY:HA2	2.39	0.57
1:B:385:LEU:HD22	1:B:424:PHE:HB3	1.86	0.57
1:A:704:LYS:HE2	1:A:722:ASP:OD1	2.05	0.56
1:A:538:THR:HG21	1:A:582:PHE:CZ	2.40	0.56
1:B:217:VAL:HG21	1:B:462:LYS:HD2	1.85	0.56
1:A:579:PRO:O	1:A:580:LEU:C	2.44	0.56
1:A:682:GLU:CD	1:A:684:ARG:HE	2.09	0.56
1:B:636:VAL:HG12	1:B:648:VAL:HG22	1.88	0.56
1:B:213:PHE:CE1	1:B:474:MET:HB3	2.40	0.56
1:B:446:LYS:NZ	1:B:446:LYS:HB2	2.21	0.55
1:B:488:GLU:OE1	1:B:491:ARG:NH1	2.40	0.55
1:A:1:SAC:O	1:A:2:GLU:HB3	2.06	0.55
1:A:443:THR:HB	1:A:451:VAL:HG13	1.88	0.55
1:B:26:LEU:HD11	1:B:104:VAL:HG11	1.88	0.55
1:A:611:ARG:HD2	1:A:616:ARG:CZ	2.35	0.55
1:B:93:ASP:OD1	1:B:95:ARG:HB2	2.07	0.55
1:B:437:SER:HB2	1:B:460:ILE:HD13	1.90	0.54
1:A:676:MET:HE3	1:A:693:GLU:HG2	1.88	0.54
1:B:552:TYR:CD1	1:B:572:THR:HB	2.42	0.54
1:A:369:VAL:HG13	4:A:1380:HOH:O	2.07	0.54
1:A:543:SER:OG	1:A:545:ASN:ND2	2.41	0.54
1:B:548:THR:HG23	4:B:1763:HOH:O	2.08	0.53
1:B:674:ARG:NH1	4:B:1516:HOH:O	2.41	0.53
1:A:545:ASN:ND2	1:A:547:TYR:CZ	2.76	0.53
1:A:559[A]:PHE:CD2	1:B:10:GLY:HA2	2.43	0.53
1:B:44:PHE:O	1:B:45:LEU:CB	2.38	0.53
1:B:12[A]:ARG:CG	4:B:1759:HOH:O	2.55	0.53
1:A:242:MET:CE	1:A:258:VAL:HG13	2.39	0.53
1:A:562:GLY:HA2	4:A:1297:HOH:O	2.07	0.53
1:A:189:GLU:HA	1:A:194:TYR:CG	2.43	0.53
1:B:12[A]:ARG:CD	4:B:1759:HOH:O	2.35	0.53
1:A:443:THR:HB	1:A:451:VAL:CG1	2.38	0.53
1:A:666:HIS:O	1:A:707:ALA:HA	2.08	0.53
1:A:520:MET:SD	1:A:608:VAL:HG12	2.49	0.53
1:B:538:THR:HB	1:B:584:LYS:HG2	1.91	0.52
1:A:659:THR:HG22	1:A:685:PRO:CD	2.39	0.52
1:B:66:THR:HG21	1:B:75:ILE:HG22	1.92	0.52
1:A:661:ARG:NH1	1:A:681:ARG:HG2	2.25	0.52
1:A:520:MET:HB2	1:A:619:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLN:HG2	4:B:1678:HOH:O	2.08	0.52
1:A:522:PHE:HZ	1:A:606:PHE:HB2	1.75	0.52
1:A:136:MET:HB3	1:A:143:ARG:HB3	1.91	0.51
1:A:518:VAL:CG1	1:A:619:LEU:HD11	2.41	0.51
1:A:648:VAL:HG11	1:A:705:LEU:HD13	1.91	0.51
1:A:611:ARG:HD2	1:A:616:ARG:NH2	2.26	0.51
1:B:31:LEU:HD22	1:B:167:TYR:HB2	1.92	0.51
1:A:654:ASN:O	1:A:686:ASN:HA	2.10	0.51
1:B:136:MET:HB2	1:B:143:ARG:HB3	1.91	0.51
1:A:659:THR:HG22	1:A:685:PRO:HD2	1.93	0.51
1:A:162:ALA:HB3	1:A:164:TRP:CZ3	2.45	0.51
1:B:676:MET:HE3	1:B:693:GLU:HG3	1.93	0.51
1:A:282:ILE:HG13	1:A:283:TYR:N	2.25	0.50
1:A:223:ARG:HD3	1:A:224:SER:N	2.26	0.50
1:A:211:VAL:HG13	1:A:467:LYS:HD2	1.93	0.50
1:A:516:SER:O	1:A:517:ASN:CB	2.60	0.50
1:A:604:LEU:HB2	1:A:625:THR:HG22	1.93	0.50
1:B:519:ASP:HB3	1:B:540:ARG:CD	2.41	0.50
1:A:289:PRO:HD3	1:A:311:TYR:HB2	1.94	0.50
1:A:437:SER:HB2	1:A:460:ILE:HD13	1.94	0.49
1:B:706:ILE:HG23	4:B:1534:HOH:O	2.12	0.49
1:A:642:VAL:HG23	1:A:727:ARG:HB2	1.93	0.49
1:A:235:LEU:HA	1:A:327:CYS:SG	2.51	0.49
1:B:14:VAL:HG23	1:B:15:PRO:HD2	1.94	0.49
1:A:475:MET:HE2	4:A:1654:HOH:O	2.12	0.49
1:A:73:LYS:HE3	1:A:176:PRO:O	2.13	0.49
1:B:65:HIS:HD2	4:B:1278:HOH:O	1.94	0.49
1:B:468:GLN:HG2	1:B:473:GLY:O	2.13	0.49
1:B:65:HIS:HE1	4:B:1462:HOH:O	1.94	0.49
1:A:529:LEU:HD11	1:A:598:LEU:CD1	2.42	0.49
1:A:297:ASP:OD1	1:A:297:ASP:N	2.44	0.49
1:A:636:VAL:HG12	1:A:648:VAL:HG22	1.94	0.48
1:A:12[B]:ARG:NH2	4:A:1366:HOH:O	2.44	0.48
1:A:635:LYS:HD2	4:A:1455:HOH:O	2.13	0.48
1:A:681:ARG:HH11	1:A:681:ARG:CB	2.22	0.48
1:B:546:ARG:HG3	1:B:546:ARG:NH1	2.29	0.48
1:A:425:GLN:HG2	4:B:1316:HOH:O	2.14	0.48
1:A:709:MET:CE	1:A:717:VAL:HG21	2.44	0.47
1:A:1:SAC:C2A	1:B:602:ALA:HB2	2.44	0.47
1:A:95:ARG:NH1	1:A:96:ARG:HH11	2.07	0.47
1:A:356:GLU:O	1:A:611:ARG:NE	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HB3	1:A:386:PRO:HD2	1.96	0.47
1:A:702:HIS:ND1	1:A:702:HIS:C	2.68	0.47
1:B:126:GLN:O	1:B:147:GLN:NE2	2.45	0.47
1:A:271:ASP:HA	1:A:308:PRO:HG2	1.97	0.47
1:A:98:LEU:HD23	1:A:164:TRP:HB2	1.96	0.47
1:B:538:THR:HG21	1:B:584:LYS:HZ2	1.80	0.47
1:A:223:ARG:NH2	1:A:292:TRP:O	2.47	0.47
1:B:140:ARG:HD2	1:B:140:ARG:N	2.30	0.47
1:B:684:ARG:O	1:B:687:SER:HB3	2.15	0.47
1:B:548:THR:CG2	1:B:613:ASN:HD22	2.06	0.47
1:A:223:ARG:HD3	1:A:224:SER:O	2.14	0.47
1:A:209:ILE:HD13	1:A:704:LYS:HB2	1.96	0.47
1:A:287:VAL:HG13	1:A:310:ARG:O	2.15	0.47
1:A:487:GLN:NE2	1:A:489:GLU:OE1	2.47	0.47
1:A:1:SAC:CB	1:B:713:SER:O	2.63	0.47
1:B:639:THR:HB	1:B:641:VAL:HG23	1.96	0.47
1:A:570:LYS:H	1:A:570:LYS:HD2	1.80	0.46
1:B:90:ARG:HB2	1:B:91:PRO:CD	2.45	0.46
1:A:349:GLN:OE1	1:A:505:PRO:HD2	2.15	0.46
1:B:674:ARG:CD	1:B:675:PRO:HD2	2.45	0.46
1:B:465:VAL:HG21	1:B:474:MET:SD	2.56	0.46
1:A:165:THR:HB	1:A:166:PRO:HD2	1.98	0.46
1:A:197:ASN:HB3	1:A:200:GLU:HB2	1.98	0.46
1:A:522:PHE:CZ	1:A:606:PHE:HB2	2.50	0.46
1:B:494:LEU:HD22	1:B:494:LEU:O	2.16	0.46
1:A:209:ILE:HG21	1:A:704:LYS:HD3	1.97	0.46
1:A:538:THR:CG2	1:A:582:PHE:CZ	2.99	0.46
1:A:72:ASN:C	1:A:72:ASN:OD1	2.55	0.45
1:A:630:PRO:O	1:A:717:VAL:HG13	2.16	0.45
1:A:648:VAL:CG1	1:A:705:LEU:HD13	2.47	0.45
1:A:282:ILE:HG13	1:A:283:TYR:H	1.80	0.45
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.98	0.45
1:A:1:SAC:H	1:B:715:ARG:H	1.65	0.45
1:B:24:ASP:HA	4:B:1519:HOH:O	2.16	0.45
1:A:52:LEU:O	1:A:53:PHE:C	2.55	0.45
1:A:519:ASP:HB2	1:A:540:ARG:HB3	1.98	0.45
1:A:600:GLU:OE1	1:A:715:ARG:NH1	2.49	0.45
1:A:536:SER:CB	1:A:584:LYS:HE2	2.46	0.45
1:A:682:GLU:OE1	1:A:684:ARG:HG3	2.16	0.45
1:B:706:ILE:HG21	4:B:1662:HOH:O	2.15	0.45
1:A:4:SER:OG	1:B:597:GLN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:HD13	1:A:474:MET:SD	2.57	0.45
1:A:727:ARG:HA	1:A:727:ARG:NH1	2.29	0.45
1:B:595:MET:HE3	1:B:598:LEU:HD11	1.97	0.45
1:A:549:ILE:CG2	1:A:610:ALA:HB1	2.47	0.45
1:B:48:THR:O	1:B:49:SER:HB3	2.16	0.45
1:A:559[B]:PHE:CD1	1:B:8:PHE:CE2	2.90	0.44
1:B:12[A]:ARG:NH2	4:B:1503:HOH:O	2.49	0.44
1:A:559[A]:PHE:CZ	1:A:599:LEU:HD13	2.52	0.44
1:A:667:LEU:HD23	1:A:676:MET:CE	2.48	0.44
1:B:553:LEU:O	1:B:570:LYS:HD2	2.17	0.44
1:A:30:GLU:HB2	1:A:169:VAL:HB	2.00	0.44
1:B:339:PHE:HA	1:B:370:TRP:O	2.17	0.44
1:A:629:ILE:HD12	1:A:630:PRO:HG2	1.98	0.44
1:A:242:MET:HE1	1:A:258:VAL:HG22	1.93	0.44
1:A:231:GLU:HA	1:A:231:GLU:OE1	2.18	0.44
1:B:529:LEU:CD2	1:B:656:LEU:HD21	2.47	0.44
1:B:641:VAL:O	1:B:642:VAL:C	2.55	0.44
1:A:569:LYS:HD2	1:A:593:GLU:OE1	2.17	0.44
1:A:29:VAL:O	1:A:29:VAL:HG23	2.18	0.44
1:A:598:LEU:HD11	1:A:627:LEU:HD13	2.00	0.43
1:B:443:THR:HB	1:B:451:VAL:CG1	2.34	0.43
1:A:1:SAC:O	1:A:2:GLU:CB	2.67	0.43
1:B:579:PRO:O	1:B:580:LEU:C	2.53	0.43
1:A:44:PHE:CZ	1:A:166:PRO:HD2	2.53	0.43
1:A:674:ARG:HH11	1:A:674:ARG:HG3	1.84	0.43
1:A:189:GLU:HA	1:A:194:TYR:CD1	2.53	0.43
1:A:310:ARG:HA	1:A:311:TYR:HA	1.72	0.43
1:A:491:ARG:HD2	4:A:1658:HOH:O	2.18	0.43
1:B:428:ALA:N	1:B:429:PRO:CD	2.82	0.43
1:A:629:ILE:HD13	1:A:714:LEU:HD11	1.99	0.43
1:A:634:ILE:HD12	1:A:720:GLU:HA	2.00	0.43
1:B:130:TRP:HA	1:B:147:GLN:O	2.18	0.43
1:A:569:LYS:HE2	1:A:589:ILE:HG13	2.01	0.43
1:A:578:GLU:O	1:A:581:SER:OG	2.22	0.43
1:A:663:VAL:HG13	1:A:709:MET:SD	2.59	0.43
1:B:377:GLU:HA	1:B:393:GLN:O	2.19	0.43
1:B:42:GLN:O	1:B:43:GLU:OE1	2.36	0.43
1:A:683:ILE:HG12	1:A:689:VAL:HG13	2.01	0.43
1:B:88:PHE:O	1:B:140:ARG:HB3	2.19	0.42
1:B:56:ARG:CD	1:B:67:ASP:O	2.67	0.42
1:B:439:LEU:HB2	1:B:456:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:PHE:CZ	1:B:585:GLU:HG2	2.54	0.42
1:B:264:ALA:HA	1:B:408:ARG:HG2	2.02	0.42
1:B:629:ILE:CG2	1:B:717:VAL:HG22	2.50	0.42
1:B:117:ILE:HG21	1:B:130:TRP:CE2	2.55	0.42
1:B:611:ARG:HB3	1:B:611:ARG:HE	1.66	0.42
1:B:184:PHE:HB3	1:B:193:VAL:HG11	2.02	0.42
1:B:310[B]:ARG:HA	1:B:311:TYR:HA	1.62	0.42
1:A:194:TYR:CE2	1:A:196:ASP:HB3	2.55	0.42
1:A:428:ALA:N	1:A:429:PRO:CD	2.83	0.42
1:A:173:SER:HA	4:A:1500:HOH:O	2.19	0.42
1:A:425:GLN:HB2	1:A:426:PHE:CD2	2.54	0.42
1:B:595:MET:HE3	1:B:598:LEU:CD1	2.50	0.41
1:B:72:ASN:ND2	4:B:1789:HOH:O	2.53	0.41
1:B:310[A]:ARG:HA	1:B:311:TYR:HA	1.66	0.41
1:B:100:ARG:HG2	1:B:119:VAL:O	2.20	0.41
1:A:661:ARG:HH12	1:A:681:ARG:HG2	1.85	0.41
1:A:559[A]:PHE:CD2	1:B:10:GLY:CA	3.03	0.41
1:B:12[A]:ARG:HG2	4:B:1759:HOH:O	2.20	0.41
1:A:659:THR:HG22	1:A:685:PRO:HD3	2.02	0.41
1:A:606:PHE:HE2	1:A:625:THR:HB	1.85	0.41
1:A:541:ASN:CB	1:A:577:LEU:HD22	2.51	0.41
1:A:696:ARG:O	1:A:697:PRO:C	2.58	0.41
1:B:538:THR:CG2	4:B:1495:HOH:O	2.69	0.41
1:B:90:ARG:HB2	1:B:91:PRO:HD2	2.03	0.41
1:B:156:LYS:HD2	1:B:181:TYR:CE2	2.55	0.41
1:B:664:TRP:CE3	1:B:677:LYS:HD2	2.55	0.41
1:B:634:ILE:HD11	1:B:707:ALA:HB2	2.02	0.41
1:B:237:THR:HG21	1:B:299:LEU:HB3	2.02	0.41
1:A:361:ASN:ND2	1:A:364:LEU:HD22	2.36	0.41
1:A:489:GLU:H	1:A:489:GLU:CD	2.24	0.40
1:B:516:SER:HB3	1:B:617:ASP:OD2	2.21	0.40
1:A:181:TYR:CD2	1:A:235:LEU:HD21	2.56	0.40
1:B:418:LYS:NZ	1:B:479:ASP:O	2.41	0.40
1:A:525:GLU:HB3	1:A:533:PHE:HB2	2.03	0.40
1:B:523:GLU:O	1:B:535:LEU:HA	2.21	0.40
1:A:81:SER:HA	1:A:146:ILE:O	2.21	0.40
1:A:77:ARG:HB3	1:A:185:ASN:HB2	2.02	0.40
1:B:529:LEU:HD12	1:B:595:MET:HE3	2.02	0.40
1:A:684:ARG:O	1:A:685:PRO: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	705/731 (96%)	668 (95%)	34 (5%)	3 (0%)	39 33
1	B	706/731 (97%)	676 (96%)	28 (4%)	2 (0%)	46 41
All	All	1411/1462 (96%)	1344 (95%)	62 (4%)	5 (0%)	39 33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	B	45	LEU
1	A	580	LEU
1	A	292	TRP
1	B	669	GLY

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	625/643 (97%)	565 (90%)	60 (10%)	10 6
1	B	627/643 (98%)	580 (92%)	47 (8%)	17 11
All	All	1252/1286 (97%)	1145 (92%)	107 (8%)	14 8

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU

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Mol	Chain	Res	Type
1	A	12[A]	ARG
1	A	12[B]	ARG
1	A	14	VAL
1	A	18	ASN
1	A	20	ASN
1	A	27	PRO
1	A	45	LEU
1	A	86	ILE
1	A	95	ARG
1	A	96	ARG
1	A	104	VAL
1	A	127	SER
1	A	136	MET
1	A	177[A]	GLU
1	A	177[B]	GLU
1	A	193	VAL
1	A	195	LEU
1	A	223	ARG
1	A	224	SER
1	A	269	LYS
1	A	270	ASP
1	A	282	ILE
1	A	287	VAL
1	A	289	PRO
1	A	290	SER
1	A	293	THR
1	A	297	ASP
1	A	340	SER
1	A	359	ASN
1	A	364	LEU
1	A	366	LYS
1	A	408	ARG
1	A	482	LYS
1	A	485	GLU
1	A	487	GLN
1	A	503	LYS
1	A	516	SER
1	A	534	LYS
1	A	543	SER
1	A	545	ASN
1	A	570	LYS
1	A	572	THR

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Mol	Chain	Res	Type
1	A	574	ASP
1	A	590	GLN
1	A	603	SER
1	A	616	ARG
1	A	618	VAL
1	A	625	THR
1	A	629	ILE
1	A	644	SER
1	A	661	ARG
1	A	674	ARG
1	A	675	PRO
1	A	678	LYS
1	A	681	ARG
1	A	684	ARG
1	A	702	HIS
1	A	704	LYS
1	A	727	ARG
1	B	14	VAL
1	B	20	ASN
1	B	25	ASP
1	B	32	GLN
1	B	42	GLN
1	B	43	GLU
1	B	47	VAL
1	B	127	SER
1	B	140	ARG
1	B	193	VAL
1	B	223	ARG
1	B	269	LYS
1	B	271	ASP
1	B	354	LEU
1	B	408	ARG
1	B	445	LYS
1	B	446	LYS
1	B	451	VAL
1	B	455	VAL
1	B	463	LEU
1	B	465	VAL
1	B	484	GLN
1	B	489	GLU
1	B	492	LEU
1	B	494	LEU

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Mol	Chain	Res	Type
1	B	498	LEU
1	B	504	LYS
1	B	507	ASN
1	B	519	ASP
1	B	538	THR
1	B	540	ARG
1	B	546	ARG
1	B	553	LEU
1	B	572	THR
1	B	575	VAL
1	B	588	LEU
1	B	589	ILE
1	B	604	LEU
1	B	623	LYS
1	B	650	VAL
1	B	659	THR
1	B	661	ARG
1	B	676	MET
1	B	687	SER
1	B	704	LYS
1	B	721	LEU
1	B	727	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	46	ASN
1	A	313	GLN
1	A	421	HIS
1	A	487	GLN
1	A	526	ASN
1	A	545	ASN
1	A	601	GLN
1	A	662	ASN
1	A	686	ASN
1	B	42	GLN
1	B	65	HIS
1	B	267	ASN
1	B	347	ASN
1	B	544	HIS
1	B	613	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	SAC	A	1	1	7,8,9	0.77	0	7,9,11	2.77	3 (42%)

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
1	SAC	A	1	1	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	SAC	C2A-C1A-N	-3.01	110.35	116.11
1	A	1	SAC	OG-CB-CA	4.11	120.38	111.04
1	A	1	SAC	OAC-C1A-C2A	4.61	130.53	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	SAC	7	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PGO	B	1203	-	4,4,4	1.45	1 (25%)	2,4,4	3.14	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGO	B	1203	-	-	0/2/2/2	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1203	PGO	C1-C2	2.71	1.57	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1203	PGO	O1-C1-C2	-4.09	101.17	110.87

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

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

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^{th} 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	707/731 (96%)	-0.02	27 (3%) 44 45	26, 43, 70, 91	4 (0%)
1	B	708/731 (96%)	-0.22	15 (2%) 67 67	23, 37, 64, 86	1 (0%)
All	All	1415/1462 (96%)	-0.12	42 (2%) 54 55	23, 40, 68, 91	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ARG	8.9
1	A	284	ALA	5.0
1	A	3	THR	4.8
1	A	6	THR	4.8
1	A	167	TYR	4.6
1	A	7	ALA	4.4
1	A	681	ARG	4.0
1	A	4	SER	3.9
1	A	270	ASP	3.9
1	B	95	ARG	3.7
1	B	686	ASN	3.6
1	B	285	TYR	3.6
1	A	285	TYR	3.6
1	B	167	TYR	3.5
1	B	582	PHE	3.5
1	A	95	ARG	3.4
1	B	8	PHE	3.2
1	B	35	VAL	3.1
1	B	33	GLY	3.0
1	A	674	ARG	2.8
1	A	661	ARG	2.7
1	A	96	ARG	2.7
1	A	684	ARG	2.7
1	A	696	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	271	ASP	2.7
1	A	656	LEU	2.6
1	B	270	ASP	2.6
1	A	545	ASN	2.6
1	B	507	ASN	2.6
1	B	127	SER	2.5
1	B	34	VAL	2.5
1	B	611	ARG	2.4
1	A	612	ILE	2.3
1	A	127	SER	2.2
1	B	681	ARG	2.2
1	B	639	THR	2.2
1	A	658	GLU	2.2
1	A	166	PRO	2.2
1	A	487	GLN	2.1
1	A	726	GLN	2.1
1	A	43	GLU	2.1
1	A	123	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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(Å^2)	Q<0.9
1	SAC	A	1	9/10	0.66	0.33	-	53,59,68,71	0

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, 95^{th} 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(Å^2)	Q<0.9
3	PGO	B	1203	5/5	0.97	0.12	2.92	39,42,46,47	0
2	CA	A	1201	1/1	0.93	0.06	-1.19	57,57,57,57	0
2	CA	B	1202	1/1	0.97	0.07	-1.60	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.