



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FRW
Title : Crystal structure of human nectin-4 extracellular fragment D1-D2
Authors : Harrison, O.J.; Jin, X.; Brasch, J.; Shapiro, L.
Deposited on : 2012-06-26
Resolution : 3.50 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

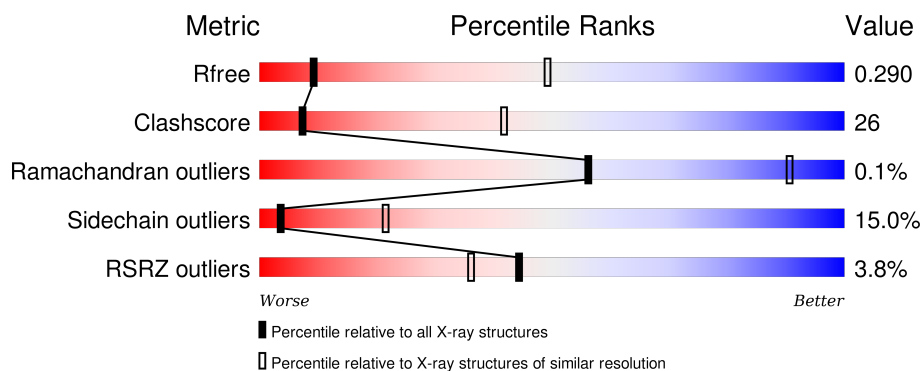
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	218	 60% 33% 5% •
1	B	218	 55% 34% 9% •
1	C	218	 61% 29% 6% •
1	D	218	 4% 60% 32% 6% •
1	E	218	 9% 56% 33% 6% 5%

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Mol	Chain	Length	Quality of chain
1	F	218	<div><div></div><div></div><div></div><div></div><div></div></div> <div>9%42%34%10%13%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9257 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 Poliovirus receptor-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1611	1002	291	313	5			
1	B	213	Total	C	N	O	S	0	0	0
			1601	996	289	311	5			
1	C	211	Total	C	N	O	S	0	0	0
			1571	978	280	308	5			
1	D	212	Total	C	N	O	S	0	0	0
			1561	973	278	305	5			
1	E	208	Total	C	N	O	S	0	0	0
			1533	954	276	298	5			
1	F	189	Total	C	N	O	S	0	0	0
			1380	860	246	269	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	HIS	-	EXPRESSION TAG	UNP Q96NY8
A	245	HIS	-	EXPRESSION TAG	UNP Q96NY8
A	246	HIS	-	EXPRESSION TAG	UNP Q96NY8
A	247	HIS	-	EXPRESSION TAG	UNP Q96NY8
A	248	HIS	-	EXPRESSION TAG	UNP Q96NY8
A	249	HIS	-	EXPRESSION TAG	UNP Q96NY8
B	244	HIS	-	EXPRESSION TAG	UNP Q96NY8
B	245	HIS	-	EXPRESSION TAG	UNP Q96NY8
B	246	HIS	-	EXPRESSION TAG	UNP Q96NY8
B	247	HIS	-	EXPRESSION TAG	UNP Q96NY8
B	248	HIS	-	EXPRESSION TAG	UNP Q96NY8
B	249	HIS	-	EXPRESSION TAG	UNP Q96NY8
C	244	HIS	-	EXPRESSION TAG	UNP Q96NY8
C	245	HIS	-	EXPRESSION TAG	UNP Q96NY8
C	246	HIS	-	EXPRESSION TAG	UNP Q96NY8
C	247	HIS	-	EXPRESSION TAG	UNP Q96NY8
C	248	HIS	-	EXPRESSION TAG	UNP Q96NY8

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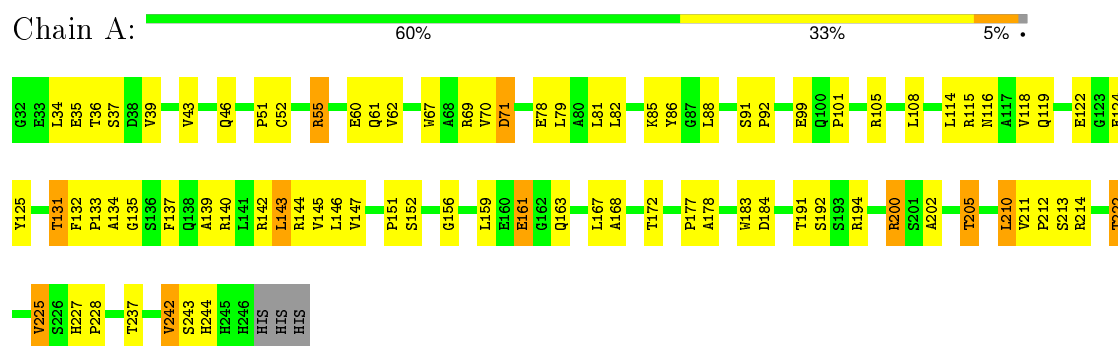
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Chain	Residue	Modelled	Actual	Comment	Reference
C	249	HIS	-	EXPRESSION TAG	UNP Q96NY8
D	244	HIS	-	EXPRESSION TAG	UNP Q96NY8
D	245	HIS	-	EXPRESSION TAG	UNP Q96NY8
D	246	HIS	-	EXPRESSION TAG	UNP Q96NY8
D	247	HIS	-	EXPRESSION TAG	UNP Q96NY8
D	248	HIS	-	EXPRESSION TAG	UNP Q96NY8
D	249	HIS	-	EXPRESSION TAG	UNP Q96NY8
E	244	HIS	-	EXPRESSION TAG	UNP Q96NY8
E	245	HIS	-	EXPRESSION TAG	UNP Q96NY8
E	246	HIS	-	EXPRESSION TAG	UNP Q96NY8
E	247	HIS	-	EXPRESSION TAG	UNP Q96NY8
E	248	HIS	-	EXPRESSION TAG	UNP Q96NY8
E	249	HIS	-	EXPRESSION TAG	UNP Q96NY8
F	244	HIS	-	EXPRESSION TAG	UNP Q96NY8
F	245	HIS	-	EXPRESSION TAG	UNP Q96NY8
F	246	HIS	-	EXPRESSION TAG	UNP Q96NY8
F	247	HIS	-	EXPRESSION TAG	UNP Q96NY8
F	248	HIS	-	EXPRESSION TAG	UNP Q96NY8
F	249	HIS	-	EXPRESSION TAG	UNP Q96NY8

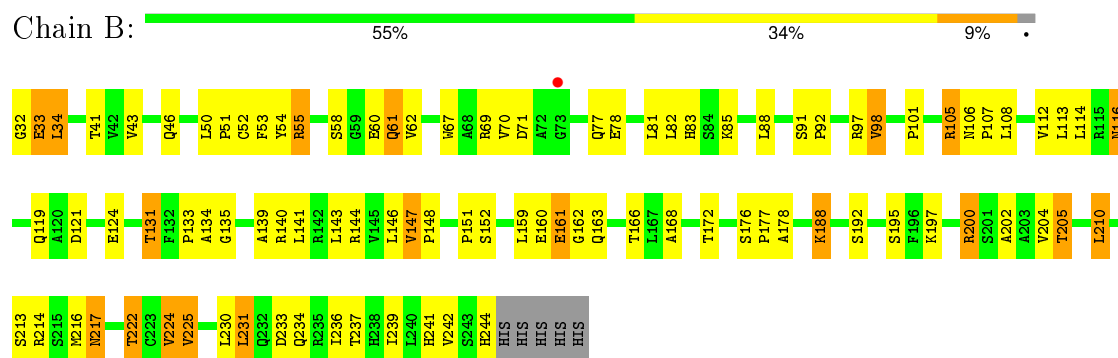
3 Residue-property plots

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.

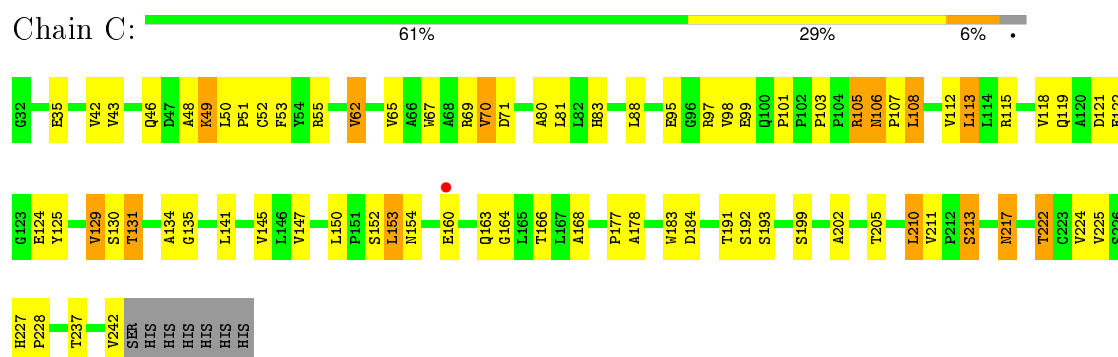
• Molecule 1: Poliovirus receptor-related protein 4



• Molecule 1: Poliovirus receptor-related protein 4



• Molecule 1: Poliovirus receptor-related protein 4



Chain D:

60% 32% 4% 6%

GLY E33 L34 E35 T36 S37 D38 V42 V43 Q46 K49 F52 F53 Y54 S58 G59 E60 V65 A66 W67 A68 R69 V70 D71 A72 G73 E74 G75 A76 Q77 E78 L79 S91 P92 A93 Y94 V98 E99 Q100 P101 P104 R105 N106 P107 L108 V112 L113 L114 R115 N116 A117 Q119 A120 D121 E124 R128 V129 S130 T131 F132 G135 Q138 A139 R140 L141 R142 V145 L146 V147 P151 N154 L159 E160 E161 T172 A173 E174 G175 S176 D184 T190 R194 K197 R200 S201 A202 A203 L210 S213 R214 S215 M216 Q219 T222 C223 V224 V225 S226 H227 L230 Q234 T237 V242 S243 H244 H1S H1S H1S H1S H1S

Chain E:

9% 56% 33% 6% 5%

GLY GLU L34 E35 T36 S37 P38 T41 V42 V43 Q46 D47 P61 C52 F53 Y54 R55 D56 D57 S58 S59 P60 D61 V62 G63 G64 V65 A66 N67 A68 A69 V70 D71 A72 G73 E74 G75 A76 L79 A80 L81 L82 H83 T86 L87 L88 H89 V90 S91 P92 A93 Y94 R97 V98 E99 Q100 P101 P102 P103 P104 N106 P107 V112 L113 L114 R115 V118 Q119 A120 D121 E124 Y125 R128 V129 S130 T131 F132 P133 Q138 A139 R140 L141 R142 L143 R144 V147 P148 P149 L150 P151 S152 L153 L159 Q163 G164 L165 T166 L167 S170 A178 T182 A183

Chain F:

9% 42% 34% 10% 13%

GLY GLU LEU GLU TS36 TS37 D38 D39 V40 V41 V42 V43 V44 A48 A49 L50 P51 C52 F53 T54 A58 A59 S60 S61 S62 S63 S64 S65 S66 S67 S68 S69 S70 S71 S72 S73 S74 S75 S76 S77 S78 S79 S80 S81 S82 S83 S84 S85 S86 S87 S88 S89 S90 S91 S92 S93 S94 S95 S96 S97 S98 P101 P102 P103 P104 R105 R106 R107 L108 L109 G110 S111 V112 L113 L114 R115 V118 Y125 V129 S130 T131 P132 P133 P134 P135 P136 P137 P138 P139 P140 P141 P142 P143 P144 P145 P146 P147 P148 P149 P150 P151 S152 S153 L154 L155 L156 L157 L158 L159 L160 L161 L162 L163 L164 L165 L166 S170 S171 S172 S173 S174 S175 S176 S177 S178 S179 S180 S181 S182 S183 S184 S185 S186 S187 S188 S189 S190 S191 S192 S193 S194 S195 S196 S197 S198 S199 S200 S201 A202 A203 V204 T205 S206 E207 F208 H209 L210 V211 P212 S213 S214 R214 T222 C223 C224 V224 V225 V226 S227 E228 L231 L232 L233 Q234 R235 L236 T237 L240 E244 E245 E246 H247 H248 H249 H250 H251 H252 H253 H254 H255 H256 H257 H258 H259 H260 H261 H262 H263 H264 H265 H266 H267 H268 H269 H270 H271 H272 H273 H274 H275 H276 H277 H278 H279 H280 H281 H282 H283 H284 H285 H286 H287 H288 H289 H290 H291 H292 H293 H294 H295 H296 H297 H298 H299 H300 H301 H302 H303 H304 H305 H306 H307 H308 H309 H310 H311 H312 H313 H314 H315 H316 H317 H318 H319 H320 H321 H322 H323 H324 H325 H326 H327 H328 H329 H330 H331 H332 H333 H334 H335 H336 H337 H338 H339 H340 H341 H342 H343 H344 H345 H346 H347 H348 H349 H350 H351 H352 H353 H354 H355 H356 H357 H358 H359 H360 H361 H362 H363 H364 H365 H366 H367 H368 H369 H370 H371 H372 H373 H374 H375 H376 H377 H378 H379 H380 H381 H382 H383 H384 H385 H386 H387 H388 H389 H390 H391 H392 H393 H394 H395 H396 H397 H398 H399 H400 H401 H402 H403 H404 H405 H406 H407 H408 H409 H410 H411 H412 H413 H414 H415 H416 H417 H418 H419 H420 H421 H422 H423 H424 H425 H426 H427 H428 H429 H430 H431 H432 H433 H434 H435 H436 H437 H438 H439 H440 H441 H442 H443 H444 H445 H446 H447 H448 H449 H450 H451 H452 H453 H454 H455 H456 H457 H458 H459 H460 H461 H462 H463 H464 H465 H466 H467 H468 H469 H470 H471 H472 H473 H474 H475 H476 H477 H478 H479 H480 H481 H482 H483 H484 H485 H486 H487 H488 H489 H490 H491 H492 H493 H494 H495 H496 H497 H498 H499 H500 H501 H502 H503 H504 H505 H506 H507 H508 H509 H510 H511 H512 H513 H514 H515 H516 H517 H518 H519 H520 H521 H522 H523 H524 H525 H526 H527 H528 H529 H530 H531 H532 H533 H534 H535 H536 H537 H538 H539 H540 H541 H542 H543 H544 H545 H546 H547 H548 H549 H550 H551 H552 H553 H554 H555 H556 H557 H558 H559 H560 H561 H562 H563 H564 H565 H566 H567 H568 H569 H570 H571 H572 H573 H574 H575 H576 H577 H578 H579 H580 H581 H582 H583 H584 H585 H586 H587 H588 H589 H590 H591 H592 H593 H594 H595 H596 H597 H598 H599 H600 H601 H602 H603 H604 H605 H606 H607 H608 H609 H610 H611 H612 H613 H614 H615 H616 H617 H618 H619 H620 H621 H622 H623 H624 H625 H626 H627 H628 H629 H630 H631 H632 H633 H634 H635 H636 H637 H638 H639 H640 H641 H642 H643 H644 H645 H646 H647 H648 H649 H650 H651 H652 H653 H654 H655 H656 H657 H658 H659 H660 H661 H662 H663 H664 H665 H666 H667 H668 H669 H670 H671 H672 H673 H674 H675 H676 H677 H678 H679 H680 H681 H682 H683 H684 H685 H686 H687 H688 H689 H690 H691 H692 H693 H694 H695 H696 H697 H698 H699 H700 H701 H702 H703 H704 H705 H706 H707 H708 H709 H710 H711 H712 H713 H714 H715 H716 H717 H718 H719 H720 H721 H722 H723 H724 H725 H726 H727 H728 H729 H730 H731 H732 H733 H734 H735 H736 H737 H738 H739 H740 H741 H742 H743 H744 H745 H746 H747 H748 H749 H750 H751 H752 H753 H754 H755 H756 H757 H758 H759 H760 H761 H762 H763 H764 H765 H766 H767 H768 H769 H770 H771 H772 H773 H774 H775 H776 H777 H778 H779 H780 H781 H782 H783 H784 H785 H786 H787 H788 H789 H790 H791 H792 H793 H794 H795 H796 H797 H798 H799 H800 H801 H802 H803 H804 H805 H806 H807 H808 H809 H810 H811 H812 H813 H814 H815 H816 H817 H818 H819 H820 H821 H822 H823 H824 H825 H826 H827 H828 H829 H830 H831 H832 H833 H834 H835 H836 H837 H838 H839 H840 H841 H842 H843 H844 H845 H846 H847 H848 H849 H850 H851 H852 H853 H854 H855 H856 H857 H858 H859 H860 H861 H862 H863 H864 H865 H866 H867 H868 H869 H870 H871 H872 H873 H874 H875 H876 H877 H878 H879 H880 H881 H882 H883 H884 H885 H886 H887 H888 H889 H890 H891 H892 H893 H894 H895 H896 H897 H898 H899 H900 H901 H902 H903 H904 H905 H906 H907 H908 H909 H910 H911 H912 H913 H914 H915 H916 H917 H918 H919 H920 H921 H922 H923 H924 H925 H926 H927 H928 H929 H930 H931 H932 H933 H934 H935 H936 H937 H938 H939 H940 H941 H942 H943 H944 H945 H946 H947 H948 H949 H950 H951 H952 H953 H954 H955 H956 H957 H958 H959 H960 H961 H962 H963 H964 H965 H966 H967 H968 H969 H970 H971 H972 H973 H974 H975 H976 H977 H978 H979 H980 H981 H982 H983 H984 H985 H986 H987 H988 H989 H990 H991 H992 H993 H994 H995 H996 H997 H998 H999

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.97Å 142.81Å 341.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.01 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-3.50) 99.4 (20.01-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.257 , 0.290 0.260 , 0.290	Depositor DCC
R_{free} test set	1334 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	96.9	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.1	EDS
Estimated twinning fraction	0.054 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.055 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 26635 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9257	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.71	0/1649	0.91	4/2251 (0.2%)
1	B	0.71	0/1639	0.86	1/2237 (0.0%)
1	C	0.70	0/1608	0.84	1/2199 (0.0%)
1	D	0.65	0/1598	0.84	1/2187 (0.0%)
1	E	0.68	1/1569 (0.1%)	0.89	4/2148 (0.2%)
1	F	0.68	1/1409 (0.1%)	0.86	3/1930 (0.2%)
All	All	0.69	2/9472 (0.0%)	0.87	14/12952 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	TRP	CD2-CE2	5.49	1.48	1.41
1	F	183	TRP	CD2-CE2	5.25	1.47	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	105	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	71	ASP	CB-CG-OD1	6.00	123.70	118.30
1	F	240	LEU	CA-CB-CG	5.74	128.49	115.30
1	B	200	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	E	97	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	55	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	200	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	E	231	LEU	CA-CB-CG	5.28	127.44	115.30
1	E	38	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	184	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	F	79	LEU	CA-CB-CG	5.12	127.09	115.30
1	F	194	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	128	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1611	0	1566	77	0
1	B	1601	0	1562	63	0
1	C	1571	0	1517	64	0
1	D	1561	0	1505	64	0
1	E	1533	0	1478	87	0
1	F	1380	0	1328	118	0
All	All	9257	0	8956	469	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 26.

All (469) 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:E:66:ALA:HB1	1:E:128:ARG:CZ	1.22	1.62
1:E:66:ALA:CB	1:E:128:ARG:CZ	2.00	1.40
1:E:66:ALA:HB1	1:E:128:ARG:NH2	1.43	1.33
1:E:101:PRO:O	1:E:105:ARG:HD3	1.38	1.19
1:E:66:ALA:CB	1:E:128:ARG:NE	2.06	1.18
1:F:153:LEU:HD23	1:F:236:ILE:HG22	1.26	1.17
1:A:131:THR:CG2	1:A:135:GLY:O	2.01	1.08
1:E:79:LEU:HG	1:E:94:TYR:CE1	1.89	1.07
1:F:51:PRO:HB3	1:F:111:SER:OG	1.55	1.06
1:F:151:PRO:HA	1:F:172:THR:O	1.56	1.05
1:F:50:LEU:HD22	1:F:141:LEU:CD1	1.88	1.03
1:A:70:VAL:HG11	1:A:140:ARG:NH1	1.72	1.03
1:E:66:ALA:HB3	1:E:128:ARG:CG	1.88	1.02
1:F:50:LEU:HD22	1:F:141:LEU:HD13	1.38	1.02
1:E:101:PRO:O	1:E:105:ARG:NH1	1.94	1.01
1:A:131:THR:HG23	1:A:135:GLY:O	1.62	0.98
1:C:101:PRO:O	1:C:105:ARG:HD3	1.63	0.97
1:F:40:VAL:HG21	1:F:50:LEU:HD23	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:LEU:HD23	1:F:236:ILE:CG2	1.95	0.96
1:E:66:ALA:HB3	1:E:128:ARG:NE	1.76	0.95
1:E:41:THR:HG23	1:E:144:ARG:HG3	1.50	0.92
1:E:81:LEU:O	1:E:88:LEU:HG	1.67	0.92
1:A:131:THR:HG22	1:A:135:GLY:O	1.68	0.92
1:F:153:LEU:CD2	1:F:236:ILE:HG22	1.99	0.92
1:F:191:THR:HB	1:F:207:GLU:O	1.70	0.92
1:F:53:PHE:HA	1:F:109:ASP:OD2	1.71	0.91
1:A:101:PRO:O	1:A:105:ARG:HD3	1.69	0.91
1:F:183:TRP:CD1	1:F:191:THR:HG21	2.09	0.88
1:E:101:PRO:O	1:E:105:ARG:CD	2.21	0.88
1:C:213:SER:O	1:C:242:VAL:HG21	1.74	0.88
1:F:51:PRO:CB	1:F:111:SER:OG	2.22	0.87
1:A:70:VAL:HG11	1:A:140:ARG:HH11	1.35	0.87
1:B:168:ALA:HB2	1:B:210:LEU:HD22	1.58	0.86
1:E:79:LEU:HG	1:E:94:TYR:CZ	2.11	0.85
1:D:120:ALA:HB2	1:D:200:ARG:HH12	1.40	0.85
1:A:70:VAL:HG21	1:A:124:GLU:CB	2.08	0.84
1:C:160:GLU:HB3	1:C:163:GLN:HE22	1.42	0.84
1:F:53:PHE:HA	1:F:109:ASP:CG	2.00	0.82
1:A:70:VAL:HG21	1:A:124:GLU:HB3	1.62	0.81
1:B:78:GLU:OE2	1:B:81:LEU:HD23	1.81	0.80
1:E:60:GLU:HB2	1:E:132:PHE:O	1.80	0.80
1:E:54:TYR:CZ	1:E:131:THR:HG21	2.16	0.80
1:F:176:SER:HB2	1:F:201:SER:HA	1.63	0.80
1:B:217:ASN:ND2	1:B:241:HIS:HA	1.95	0.80
1:C:49:LYS:HA	1:C:113:LEU:HD12	1.63	0.79
1:A:91:SER:OG	1:A:92:PRO:HD2	1.81	0.79
1:A:194:ARG:NH1	1:B:148:PRO:O	2.14	0.79
1:A:70:VAL:CG1	1:A:140:ARG:NH1	2.45	0.79
1:F:151:PRO:HG3	1:F:173:ALA:HB2	1.65	0.79
1:A:172:THR:HG23	1:A:205:THR:HG22	1.66	0.78
1:E:54:TYR:CE1	1:E:131:THR:HG21	2.18	0.78
1:F:185:THR:HG22	1:F:186:GLU:H	1.48	0.78
1:B:70:VAL:CG2	1:B:124:GLU:HB3	2.13	0.78
1:F:151:PRO:HG2	1:F:225:VAL:HG11	1.66	0.77
1:E:66:ALA:CB	1:E:128:ARG:NH2	2.31	0.77
1:D:216:MET:HA	1:D:219:GLN:HG3	1.65	0.77
1:F:53:PHE:CE2	1:F:108:LEU:HB3	2.20	0.76
1:F:105:ARG:HH12	1:F:110:GLY:HA3	1.51	0.76
1:E:66:ALA:HB3	1:E:128:ARG:HG3	1.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:PRO:CA	1:F:111:SER:OG	2.34	0.75
1:F:82:LEU:HD21	1:F:112:VAL:HG23	1.67	0.74
1:F:194:ARG:CG	1:F:194:ARG:HH11	1.99	0.74
1:E:90:VAL:HG21	1:E:94:TYR:O	1.87	0.74
1:B:222:THR:HG22	1:B:237:THR:HG23	1.68	0.74
1:B:147:VAL:HG13	1:B:176:SER:HB3	1.68	0.74
1:F:53:PHE:HD2	1:F:108:LEU:HD23	1.51	0.74
1:B:43:VAL:HG22	1:B:46:GLN:HG2	1.69	0.73
1:B:230:LEU:HD21	1:B:233:ASP:HA	1.70	0.73
1:F:80:ALA:HB3	1:F:98:VAL:HG11	1.71	0.73
1:D:121:ASP:OD1	1:D:145:VAL:HG21	1.87	0.73
1:E:60:GLU:CB	1:E:132:PHE:O	2.37	0.73
1:F:165:LEU:HB3	1:F:211:VAL:HG13	1.70	0.73
1:F:50:LEU:HD22	1:F:141:LEU:HD11	1.71	0.72
1:E:66:ALA:HB3	1:E:128:ARG:CD	2.19	0.72
1:A:70:VAL:CG2	1:A:124:GLU:CB	2.67	0.72
1:F:101:PRO:O	1:F:105:ARG:HD3	1.88	0.72
1:D:161:GLU:HA	1:D:161:GLU:OE2	1.88	0.72
1:E:64:GLN:HE21	1:E:81:LEU:HD21	1.53	0.72
1:B:69:ARG:HG2	1:B:77:GLN:HB3	1.73	0.71
1:E:232:GLN:NE2	1:E:232:GLN:HA	2.05	0.71
1:C:70:VAL:CG2	1:C:124:GLU:HB3	2.20	0.71
1:D:65:VAL:HG22	1:D:129:VAL:HG23	1.73	0.71
1:C:131:THR:HG23	1:C:135:GLY:O	1.91	0.71
1:E:224:VAL:HG23	1:E:224:VAL:O	1.91	0.70
1:F:153:LEU:CD2	1:F:236:ILE:CG2	2.62	0.70
1:E:41:THR:HG23	1:E:144:ARG:CG	2.22	0.70
1:D:159:LEU:O	1:D:242:VAL:HA	1.91	0.70
1:F:194:ARG:HG2	1:F:194:ARG:HH11	1.56	0.70
1:E:65:VAL:O	1:E:81:LEU:HD12	1.91	0.69
1:F:183:TRP:HD1	1:F:191:THR:HG21	1.55	0.69
1:D:54:TYR:CE2	1:D:131:THR:HG21	2.28	0.69
1:E:51:PRO:HD2	1:E:141:LEU:HD22	1.73	0.69
1:A:70:VAL:HG22	1:A:124:GLU:C	2.13	0.68
1:D:69:ARG:NH1	1:D:94:TYR:OH	2.27	0.68
1:C:65:VAL:HG22	1:C:129:VAL:HG22	1.76	0.68
1:F:151:PRO:CA	1:F:172:THR:O	2.39	0.68
1:A:70:VAL:CG1	1:A:140:ARG:HH12	2.05	0.68
1:F:103:PRO:HA	1:F:105:ARG:HG3	1.76	0.68
1:E:101:PRO:C	1:E:105:ARG:HD3	2.13	0.67
1:F:53:PHE:CD2	1:F:108:LEU:HD23	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG23	1:C:124:GLU:HB3	1.74	0.67
1:E:66:ALA:HB3	1:E:128:ARG:HG2	1.76	0.66
1:E:178:ALA:HB2	1:E:202:ALA:HB3	1.77	0.66
1:C:98:VAL:HG13	1:C:112:VAL:CG1	2.26	0.66
1:A:70:VAL:CG2	1:A:124:GLU:HB2	2.26	0.66
1:A:168:ALA:HB2	1:A:210:LEU:HD22	1.76	0.66
1:C:50:LEU:N	1:C:50:LEU:CD1	2.60	0.65
1:A:70:VAL:HG21	1:A:124:GLU:HB2	1.79	0.65
1:F:191:THR:CB	1:F:207:GLU:O	2.44	0.65
1:B:131:THR:OG1	1:B:134:ALA:HB3	1.96	0.65
1:B:62:VAL:HG13	1:B:108:LEU:HG	1.77	0.65
1:F:192:SER:OG	1:F:207:GLU:HB2	1.97	0.64
1:E:81:LEU:O	1:E:88:LEU:CG	2.42	0.64
1:B:34:LEU:HD13	1:B:139:ALA:HB2	1.79	0.64
1:C:80:ALA:HB1	1:C:88:LEU:HD11	1.79	0.64
1:F:50:LEU:CD2	1:F:141:LEU:HD13	2.20	0.64
1:F:37:SER:HB2	1:F:51:PRO:HD2	1.80	0.64
1:F:109:ASP:OD2	1:F:109:ASP:C	2.36	0.64
1:A:39:VAL:HG23	1:A:142:ARG:O	1.98	0.64
1:D:69:ARG:NH2	1:D:120:ALA:O	2.31	0.63
1:F:94:TYR:HB3	1:F:98:VAL:HG23	1.79	0.63
1:F:80:ALA:HB2	1:F:90:VAL:HG23	1.80	0.63
1:C:50:LEU:HD12	1:C:50:LEU:N	2.13	0.63
1:F:187:VAL:HG23	1:F:208:PHE:CZ	2.34	0.63
1:D:174:GLU:HG3	1:D:202:ALA:O	1.99	0.63
1:F:151:PRO:CG	1:F:173:ALA:HB2	2.29	0.62
1:D:116:ASN:O	1:D:118:VAL:HG23	1.99	0.62
1:D:118:VAL:HG12	1:D:119:GLN:N	2.14	0.62
1:F:40:VAL:HG21	1:F:50:LEU:CD2	2.25	0.62
1:F:178:ALA:HB2	1:F:202:ALA:HB3	1.82	0.62
1:E:153:LEU:HD21	1:E:238:HIS:HB2	1.82	0.62
1:E:91:SER:HB3	1:E:92:PRO:HD2	1.81	0.62
1:C:217:ASN:HD21	1:C:242:VAL:HB	1.63	0.62
1:A:52:CYS:HB2	1:A:67:TRP:CZ2	2.35	0.61
1:B:168:ALA:HB2	1:B:210:LEU:CD2	2.29	0.61
1:B:70:VAL:HG23	1:B:124:GLU:HB3	1.81	0.61
1:B:172:THR:HG23	1:B:205:THR:HG22	1.82	0.61
1:F:80:ALA:CB	1:F:98:VAL:HG11	2.31	0.61
1:A:82:LEU:HB3	1:A:88:LEU:HD12	1.83	0.61
1:F:51:PRO:HA	1:F:111:SER:OG	2.01	0.61
1:F:42:VAL:HG21	1:F:48:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:PRO:O	1:B:105:ARG:NH1	2.33	0.61
1:A:70:VAL:CG2	1:A:124:GLU:C	2.69	0.60
1:F:79:LEU:HD22	1:F:94:TYR:CZ	2.36	0.60
1:A:99:GLU:OE2	1:A:115:ARG:HD2	2.01	0.60
1:C:99:GLU:OE1	1:C:115:ARG:HD2	2.01	0.60
1:A:70:VAL:HG22	1:A:124:GLU:O	2.02	0.60
1:D:184:ASP:O	1:D:222:THR:HG23	2.01	0.60
1:F:191:THR:HA	1:F:207:GLU:O	2.01	0.60
1:E:232:GLN:HE21	1:E:232:GLN:HA	1.64	0.60
1:A:34:LEU:HD23	1:A:139:ALA:HB2	1.83	0.60
1:A:43:VAL:HG23	1:A:46:GLN:HG2	1.83	0.60
1:D:43:VAL:HG22	1:D:46:GLN:HG2	1.82	0.60
1:E:61:GLN:HE22	1:E:107:PRO:HB2	1.65	0.60
1:A:79:LEU:O	1:A:91:SER:HB3	2.02	0.60
1:F:151:PRO:HG3	1:F:173:ALA:CB	2.32	0.60
1:E:98:VAL:HG13	1:E:112:VAL:HG11	1.83	0.59
1:E:98:VAL:HG13	1:E:112:VAL:CG1	2.32	0.59
1:E:34:LEU:HD21	1:E:129:VAL:HG11	1.85	0.59
1:C:51:PRO:HD2	1:C:141:LEU:HD22	1.84	0.59
1:F:50:LEU:CD2	1:F:141:LEU:CD1	2.74	0.59
1:B:53:PHE:CE2	1:B:55:ARG:HD2	2.37	0.59
1:C:106:ASN:OD1	1:C:108:LEU:CD1	2.51	0.59
1:C:118:VAL:HG12	1:C:119:GLN:N	2.18	0.59
1:C:98:VAL:CG1	1:C:112:VAL:CG1	2.81	0.59
1:F:64:GLN:O	1:F:129:VAL:CG2	2.51	0.58
1:F:80:ALA:HB2	1:F:98:VAL:HG21	1.84	0.58
1:E:230:LEU:HD21	1:E:234:GLN:NE2	2.18	0.58
1:D:54:TYR:O	1:D:108:LEU:HD23	2.04	0.58
1:D:119:GLN:O	1:D:120:ALA:HB3	2.03	0.58
1:D:161:GLU:OE1	1:D:214:ARG:HG2	2.04	0.58
1:B:61:GLN:NE2	1:B:62:VAL:H	2.02	0.58
1:B:178:ALA:HB2	1:B:202:ALA:HB3	1.85	0.58
1:F:183:TRP:CD1	1:F:191:THR:CG2	2.85	0.58
1:B:121:ASP:O	1:B:143:LEU:HD23	2.04	0.58
1:B:50:LEU:N	1:B:50:LEU:HD12	2.18	0.58
1:F:50:LEU:HD13	1:F:141:LEU:HD11	1.86	0.57
1:F:40:VAL:CG2	1:F:50:LEU:HD23	2.29	0.57
1:F:53:PHE:CA	1:F:109:ASP:CG	2.72	0.57
1:A:227:HIS:CG	1:A:228:PRO:HD2	2.38	0.57
1:E:118:VAL:HG12	1:E:119:GLN:N	2.19	0.57
1:B:98:VAL:HG22	1:B:112:VAL:CG1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:HB3	1:D:77:GLN:HB3	1.85	0.57
1:E:61:GLN:NE2	1:E:107:PRO:HB2	2.20	0.57
1:B:231:LEU:CD2	1:B:231:LEU:H	2.18	0.57
1:B:160:GLU:HG2	1:B:162:GLY:H	1.69	0.57
1:E:43:VAL:HG13	1:E:46:GLN:HG3	1.86	0.57
1:E:64:GLN:HG2	1:E:81:LEU:HD11	1.87	0.57
1:B:50:LEU:N	1:B:50:LEU:CD1	2.68	0.57
1:F:227:HIS:CE1	1:F:228:PRO:O	2.58	0.57
1:F:103:PRO:CB	1:F:104:PRO:HA	2.35	0.56
1:F:194:ARG:O	1:F:204:VAL:HG23	2.04	0.56
1:B:131:THR:HG23	1:B:135:GLY:O	2.05	0.56
1:D:100:GLN:CG	1:D:105:ARG:HD3	2.35	0.56
1:F:231:LEU:H	1:F:231:LEU:HD12	1.69	0.56
1:F:194:ARG:HD3	1:F:195:SER:H	1.69	0.56
1:F:79:LEU:HD22	1:F:94:TYR:CE2	2.40	0.56
1:E:151:PRO:HG3	1:E:225:VAL:HG11	1.86	0.56
1:D:34:LEU:HD21	1:D:52:CYS:SG	2.46	0.56
1:A:184:ASP:O	1:A:222:THR:HG23	2.05	0.56
1:B:163:GLN:HG3	1:B:166:THR:HG21	1.87	0.56
1:F:185:THR:HG22	1:F:186:GLU:N	2.19	0.56
1:C:106:ASN:OD1	1:C:107:PRO:HD2	2.06	0.56
1:A:37:SER:HB2	1:A:51:PRO:HG2	1.88	0.56
1:F:149:PRO:HB2	1:F:173:ALA:HB1	1.87	0.56
1:D:210:LEU:HD23	1:D:210:LEU:O	2.06	0.55
1:D:214:ARG:NH2	1:D:244:HIS:CD2	2.74	0.55
1:B:146:LEU:HD22	1:B:177:PRO:HD3	1.88	0.55
1:B:161:GLU:OE1	1:B:214:ARG:NH1	2.39	0.55
1:B:82:LEU:O	1:B:82:LEU:HD12	2.07	0.55
1:F:160:GLU:O	1:F:212:PRO:HG2	2.07	0.54
1:E:159:LEU:HD22	1:E:166:THR:OG1	2.07	0.54
1:C:35:GLU:OE1	1:C:55:ARG:NH1	2.40	0.54
1:A:43:VAL:CG2	1:A:46:GLN:HG2	2.38	0.54
1:C:217:ASN:ND2	1:C:242:VAL:HB	2.23	0.54
1:B:112:VAL:HG12	1:B:113:LEU:N	2.23	0.54
1:A:214:ARG:NH1	1:A:242:VAL:O	2.39	0.54
1:D:91:SER:HB2	1:D:92:PRO:HD2	1.88	0.54
1:D:161:GLU:OE2	1:D:161:GLU:CA	2.54	0.54
1:B:151:PRO:HB3	1:B:225:VAL:HG11	1.90	0.54
1:E:66:ALA:HB1	1:E:128:ARG:NH1	2.07	0.54
1:D:230:LEU:HD21	1:D:234:GLN:HG2	1.91	0.54
1:D:106:ASN:OD1	1:D:107:PRO:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LEU:HD12	1:E:170:SER:O	2.08	0.53
1:C:222:THR:HB	1:C:237:THR:OG1	2.08	0.53
1:C:122:GLU:HG3	1:C:145:VAL:H	1.73	0.53
1:F:82:LEU:HD12	1:F:82:LEU:O	2.07	0.53
1:A:131:THR:CG2	1:A:134:ALA:HB3	2.39	0.53
1:B:61:GLN:HE21	1:B:62:VAL:H	1.57	0.53
1:D:222:THR:HB	1:D:237:THR:HG23	1.91	0.53
1:D:34:LEU:HD12	1:D:129:VAL:CG1	2.38	0.53
1:D:227:HIS:HB3	1:D:230:LEU:HB2	1.91	0.53
1:F:161:GLU:CB	1:F:244:HIS:HA	2.38	0.52
1:A:131:THR:HG23	1:A:134:ALA:HB3	1.92	0.52
1:C:62:VAL:HG11	1:C:108:LEU:HA	1.91	0.52
1:F:191:THR:CA	1:F:207:GLU:O	2.57	0.52
1:F:165:LEU:HD12	1:F:209:HIS:HB3	1.91	0.52
1:D:36:THR:HG21	1:D:139:ALA:HB1	1.90	0.52
1:A:70:VAL:CG2	1:A:124:GLU:O	2.58	0.52
1:A:35:GLU:OE2	1:A:55:ARG:NE	2.43	0.52
1:C:108:LEU:HD12	1:C:108:LEU:H	1.75	0.52
1:D:131:THR:O	1:D:132:PHE:HD2	1.93	0.52
1:C:118:VAL:HG12	1:C:119:GLN:H	1.75	0.52
1:F:187:VAL:HG23	1:F:208:PHE:CE2	2.44	0.52
1:B:32:GLY:HA2	1:B:54:TYR:OH	2.11	0.51
1:F:82:LEU:HD21	1:F:112:VAL:CG2	2.37	0.51
1:F:194:ARG:CD	1:F:195:SER:H	2.22	0.51
1:D:34:LEU:HD12	1:D:129:VAL:HG11	1.92	0.51
1:C:141:LEU:HD12	1:C:141:LEU:C	2.31	0.51
1:B:52:CYS:HB2	1:B:67:TRP:CZ2	2.45	0.51
1:B:112:VAL:CG1	1:B:113:LEU:N	2.73	0.51
1:A:159:LEU:O	1:A:242:VAL:HA	2.11	0.51
1:F:184:ASP:O	1:F:185:THR:OG1	2.28	0.51
1:F:37:SER:HB3	1:F:141:LEU:HD22	1.93	0.50
1:D:151:PRO:HG3	1:D:225:VAL:HG21	1.93	0.50
1:A:60:GLU:HB3	1:A:133:PRO:HD2	1.93	0.50
1:F:151:PRO:CB	1:F:173:ALA:HB2	2.42	0.50
1:E:128:ARG:HA	1:E:138:GLN:HB3	1.94	0.50
1:C:98:VAL:CG1	1:C:112:VAL:HG11	2.42	0.50
1:D:197:LYS:NZ	1:D:202:ALA:HB2	2.27	0.50
1:D:176:SER:HB2	1:D:201:SER:HA	1.92	0.50
1:D:131:THR:C	1:D:132:PHE:CD2	2.85	0.50
1:E:232:GLN:HE21	1:E:232:GLN:CA	2.23	0.50
1:D:131:THR:O	1:D:132:PHE:CD2	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ALA:HB3	1:E:128:ARG:CZ	2.13	0.49
1:A:70:VAL:HG12	1:A:140:ARG:HH12	1.75	0.49
1:F:103:PRO:HB3	1:F:104:PRO:HA	1.94	0.49
1:A:213:SER:O	1:A:242:VAL:HG21	2.12	0.49
1:B:151:PRO:HB2	1:B:236:ILE:HD11	1.94	0.49
1:C:184:ASP:O	1:C:222:THR:HG23	2.13	0.49
1:E:69:ARG:HH22	1:E:121:ASP:HA	1.77	0.49
1:C:43:VAL:HG22	1:C:46:GLN:HG2	1.94	0.49
1:F:65:VAL:HA	1:F:129:VAL:HG23	1.94	0.49
1:E:114:LEU:HD21	1:E:121:ASP:OD1	2.12	0.49
1:E:227:HIS:CG	1:E:228:PRO:HD2	2.47	0.49
1:C:227:HIS:CG	1:C:228:PRO:HD2	2.47	0.49
1:B:195:SER:OG	1:B:204:VAL:HG22	2.13	0.49
1:D:52:CYS:HB2	1:D:67:TRP:CZ2	2.47	0.49
1:A:61:GLN:HG3	1:A:62:VAL:N	2.26	0.49
1:F:105:ARG:HH12	1:F:110:GLY:CA	2.24	0.49
1:A:52:CYS:HB2	1:A:67:TRP:HZ2	1.75	0.49
1:E:69:ARG:NH2	1:E:125:TYR:OH	2.45	0.49
1:C:211:VAL:HG23	1:C:211:VAL:O	2.11	0.49
1:C:106:ASN:OD1	1:C:108:LEU:HD12	2.13	0.49
1:A:99:GLU:OE2	1:A:115:ARG:CD	2.61	0.48
1:A:151:PRO:HG3	1:A:225:VAL:HG11	1.95	0.48
1:B:159:LEU:O	1:B:242:VAL:HA	2.13	0.48
1:C:183:TRP:CD1	1:C:191:THR:HG21	2.49	0.48
1:C:69:ARG:NH1	1:C:125:TYR:OH	2.46	0.48
1:E:51:PRO:HD2	1:E:141:LEU:CD2	2.42	0.48
1:F:194:ARG:NH1	1:F:194:ARG:HG2	2.27	0.48
1:A:211:VAL:O	1:A:211:VAL:HG23	2.11	0.48
1:E:79:LEU:CG	1:E:94:TYR:CZ	2.91	0.48
1:D:174:GLU:HG3	1:D:203:ALA:HB2	1.95	0.48
1:B:60:GLU:HB3	1:B:133:PRO:HD2	1.96	0.48
1:F:153:LEU:HB2	1:F:236:ILE:HG21	1.94	0.48
1:F:194:ARG:HG3	1:F:194:ARG:HH11	1.78	0.48
1:C:51:PRO:HD2	1:C:141:LEU:CD2	2.44	0.48
1:F:222:THR:HB	1:F:237:THR:HB	1.96	0.48
1:B:188:LYS:NZ	1:B:188:LYS:HB3	2.28	0.48
1:A:35:GLU:OE2	1:A:55:ARG:HD2	2.14	0.48
1:E:60:GLU:CG	1:E:132:PHE:O	2.62	0.48
1:E:151:PRO:HG3	1:E:225:VAL:CG1	2.43	0.48
1:F:51:PRO:HA	1:F:111:SER:HA	1.95	0.48
1:D:118:VAL:HG12	1:D:119:GLN:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:HG12	1:C:113:LEU:N	2.29	0.48
1:E:224:VAL:O	1:E:224:VAL:CG2	2.61	0.47
1:E:239:ILE:H	1:E:239:ILE:HD12	1.78	0.47
1:A:143:LEU:CD2	1:A:145:VAL:HG23	2.44	0.47
1:B:51:PRO:HD2	1:B:141:LEU:HD22	1.95	0.47
1:E:159:LEU:HD21	1:E:167:LEU:O	2.13	0.47
1:A:222:THR:HB	1:A:237:THR:OG1	2.14	0.47
1:F:147:VAL:HG13	1:F:176:SER:H	1.78	0.47
1:E:34:LEU:CD2	1:E:129:VAL:HG11	2.44	0.47
1:F:40:VAL:CG2	1:F:50:LEU:CD2	2.91	0.47
1:F:36:THR:HA	1:F:51:PRO:O	2.15	0.47
1:F:48:ALA:HB3	1:F:114:LEU:HB2	1.96	0.47
1:E:69:ARG:HB2	1:E:124:GLU:O	2.15	0.47
1:F:52:CYS:HB2	1:F:67:TRP:CZ2	2.50	0.47
1:C:153:LEU:HG	1:C:154:ASN:N	2.29	0.47
1:B:91:SER:HB2	1:B:92:PRO:HD2	1.97	0.47
1:F:105:ARG:NH1	1:F:110:GLY:HA3	2.25	0.47
1:C:52:CYS:HB2	1:C:67:TRP:CZ2	2.49	0.46
1:E:230:LEU:CD2	1:E:234:GLN:NE2	2.78	0.46
1:C:81:LEU:HD12	1:C:81:LEU:C	2.35	0.46
1:E:52:CYS:HB2	1:E:67:TRP:CZ2	2.51	0.46
1:D:69:ARG:HH12	1:D:94:TYR:HH	1.59	0.46
1:F:69:ARG:HB3	1:F:125:TYR:CE1	2.50	0.46
1:B:83:HIS:NE2	1:C:83:HIS:NE2	2.63	0.46
1:F:42:VAL:HG21	1:F:48:ALA:CB	2.45	0.46
1:A:161:GLU:HG3	1:A:214:ARG:HB2	1.98	0.46
1:B:32:GLY:C	1:B:33:GLU:HG2	2.34	0.46
1:A:131:THR:HG21	1:A:137:PHE:CE2	2.51	0.46
1:E:79:LEU:CG	1:E:94:TYR:CE1	2.81	0.46
1:D:120:ALA:HB2	1:D:200:ARG:NH1	2.21	0.46
1:B:224:VAL:HG22	1:B:224:VAL:O	2.16	0.46
1:D:141:LEU:HD12	1:D:141:LEU:C	2.36	0.46
1:B:231:LEU:N	1:B:231:LEU:CD2	2.78	0.46
1:F:69:ARG:HB3	1:F:125:TYR:CD1	2.51	0.46
1:B:151:PRO:HG2	1:B:234:GLN:HG2	1.96	0.46
1:E:34:LEU:O	1:E:36:THR:HG22	2.15	0.46
1:B:83:HIS:CD2	1:C:83:HIS:HE2	2.34	0.46
1:A:62:VAL:HG13	1:A:108:LEU:HG	1.98	0.45
1:F:233:ASP:N	1:F:233:ASP:OD1	2.46	0.45
1:D:100:GLN:HG3	1:D:101:PRO:HD2	1.97	0.45
1:A:69:ARG:HG3	1:A:125:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:THR:OG1	1:F:224:VAL:HG13	2.16	0.45
1:B:82:LEU:HB3	1:B:88:LEU:HD12	1.97	0.45
1:C:103:PRO:HA	1:C:105:ARG:HG3	1.98	0.45
1:E:151:PRO:HB2	1:E:236:ILE:HD11	1.98	0.45
1:C:164:GLY:O	1:C:166:THR:HG23	2.16	0.45
1:F:176:SER:HA	1:F:177:PRO:C	2.37	0.45
1:B:147:VAL:HG22	1:B:147:VAL:O	2.17	0.45
1:D:131:THR:HG23	1:D:135:GLY:O	2.16	0.45
1:A:36:THR:HG21	1:A:139:ALA:HB1	1.98	0.45
1:B:53:PHE:HD2	1:B:55:ARG:HH11	1.62	0.45
1:A:61:GLN:HA	1:A:108:LEU:HD11	1.98	0.45
1:E:42:VAL:HG22	1:E:143:LEU:HD21	1.99	0.45
1:B:231:LEU:HD23	1:B:231:LEU:N	2.32	0.45
1:E:195:SER:HA	1:E:204:VAL:HA	1.99	0.45
1:B:34:LEU:CD2	1:B:34:LEU:C	2.85	0.44
1:F:183:TRP:CZ3	1:F:223:CYS:HB3	2.51	0.44
1:E:36:THR:HG21	1:E:139:ALA:HB1	1.98	0.44
1:A:156:GLY:HA2	1:A:167:LEU:HD23	2.00	0.44
1:C:69:ARG:HH12	1:C:121:ASP:HA	1.83	0.44
1:D:118:VAL:CG1	1:D:119:GLN:N	2.80	0.44
1:D:141:LEU:HD12	1:D:141:LEU:O	2.17	0.44
1:A:163:GLN:O	1:A:212:PRO:HD2	2.18	0.44
1:C:242:VAL:O	1:C:242:VAL:HG12	2.18	0.44
1:C:131:THR:OG1	1:C:134:ALA:HB3	2.17	0.44
1:E:79:LEU:O	1:E:91:SER:OG	2.35	0.44
1:D:98:VAL:CG1	1:D:112:VAL:HG11	2.48	0.44
1:D:119:GLN:HG3	1:D:119:GLN:O	2.18	0.44
1:F:234:GLN:HE21	1:F:234:GLN:N	2.16	0.44
1:E:41:THR:HG23	1:E:144:ARG:CD	2.48	0.44
1:D:174:GLU:CG	1:D:203:ALA:HB2	2.47	0.44
1:F:68:ALA:HB2	1:F:78:GLU:OE2	2.18	0.44
1:D:58:SER:O	1:D:60:GLU:N	2.51	0.44
1:C:98:VAL:HG13	1:C:112:VAL:HG11	2.00	0.43
1:F:65:VAL:HA	1:F:129:VAL:CG2	2.48	0.43
1:A:116:ASN:O	1:A:118:VAL:HG23	2.17	0.43
1:B:213:SER:O	1:B:216:MET:HG2	2.18	0.43
1:E:79:LEU:HG	1:E:94:TYR:CD1	2.49	0.43
1:E:34:LEU:HD21	1:E:129:VAL:CG1	2.46	0.43
1:E:118:VAL:CG1	1:E:119:GLN:N	2.81	0.43
1:C:168:ALA:HB2	1:C:210:LEU:HD22	2.00	0.43
1:D:94:TYR:HB3	1:D:98:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LEU:HA	1:C:150:LEU:HD23	1.76	0.43
1:C:49:LYS:HA	1:C:113:LEU:CD1	2.43	0.43
1:A:178:ALA:HB2	1:A:202:ALA:HB3	2.00	0.43
1:F:235:ARG:O	1:F:235:ARG:HG3	2.18	0.43
1:F:36:THR:HG21	1:F:139:ALA:HB1	1.99	0.43
1:F:151:PRO:HG3	1:F:225:VAL:HG21	2.00	0.43
1:C:49:LYS:C	1:C:50:LEU:HD12	2.38	0.43
1:F:103:PRO:CB	1:F:104:PRO:CA	2.97	0.43
1:F:65:VAL:HB	1:F:82:LEU:O	2.18	0.43
1:F:96:GLY:O	1:F:115:ARG:NH2	2.52	0.43
1:D:71:ASP:HB2	1:D:75:GLY:O	2.18	0.43
1:A:118:VAL:HG12	1:A:119:GLN:N	2.33	0.43
1:C:163:GLN:HB3	1:C:166:THR:HG21	2.01	0.43
1:A:177:PRO:CG	1:A:228:PRO:HG2	2.49	0.43
1:B:222:THR:HG22	1:B:237:THR:CG2	2.42	0.42
1:A:146:LEU:CD2	1:A:177:PRO:HD3	2.48	0.42
1:E:97:ARG:NH1	1:E:115:ARG:O	2.50	0.42
1:E:143:LEU:HD23	1:E:144:ARG:N	2.35	0.42
1:C:49:LYS:HD3	1:C:113:LEU:CD1	2.49	0.42
1:D:119:GLN:O	1:D:120:ALA:CB	2.66	0.42
1:B:239:ILE:HD12	1:B:241:HIS:HE2	1.85	0.42
1:D:49:LYS:HD2	1:D:113:LEU:HD11	2.01	0.42
1:F:186:GLU:N	1:F:186:GLU:OE2	2.51	0.42
1:C:177:PRO:CG	1:C:228:PRO:HG2	2.49	0.42
1:C:42:VAL:HG11	1:C:48:ALA:HB2	2.01	0.42
1:F:50:LEU:CD2	1:F:141:LEU:HD11	2.44	0.42
1:D:216:MET:HA	1:D:219:GLN:CG	2.44	0.42
1:B:119:GLN:CD	1:B:147:VAL:HG11	2.39	0.42
1:A:143:LEU:HD21	1:A:145:VAL:HG23	2.00	0.42
1:E:47:ASP:OD1	1:E:115:ARG:HG3	2.19	0.42
1:C:49:LYS:HB2	1:C:113:LEU:HD11	2.02	0.42
1:A:81:LEU:HD12	1:A:81:LEU:C	2.40	0.42
1:B:106:ASN:OD1	1:B:107:PRO:HD2	2.20	0.42
1:D:214:ARG:CZ	1:D:244:HIS:CD2	3.02	0.42
1:E:182:THR:HB	1:E:224:VAL:CG2	2.50	0.42
1:C:53:PHE:CE1	1:C:108:LEU:HB2	2.55	0.42
1:D:36:THR:CG2	1:D:139:ALA:HB1	2.50	0.42
1:D:65:VAL:HG22	1:D:129:VAL:CG2	2.46	0.42
1:C:35:GLU:OE1	1:C:55:ARG:HG2	2.19	0.42
1:A:35:GLU:CD	1:A:55:ARG:HE	2.22	0.42
1:F:234:GLN:HE21	1:F:234:GLN:CA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:HD3	1:A:86:TYR:CZ	2.55	0.42
1:A:70:VAL:HG23	1:A:124:GLU:HB2	1.99	0.41
1:A:70:VAL:CG2	1:A:124:GLU:HB3	2.38	0.41
1:F:53:PHE:HE2	1:F:108:LEU:HB3	1.77	0.41
1:A:91:SER:OG	1:A:92:PRO:CD	2.61	0.41
1:A:177:PRO:HD2	1:A:227:HIS:CE1	2.55	0.41
1:B:151:PRO:HG3	1:B:225:VAL:HG11	2.01	0.41
1:E:114:LEU:HD21	1:E:121:ASP:CG	2.40	0.41
1:F:91:SER:HB2	1:F:92:PRO:HD2	2.02	0.41
1:A:132:PHE:CD2	1:A:132:PHE:N	2.88	0.41
1:F:153:LEU:CD2	1:F:236:ILE:HG21	2.49	0.41
1:C:113:LEU:HA	1:C:113:LEU:HD12	1.74	0.41
1:F:159:LEU:HD23	1:F:166:THR:HB	2.02	0.41
1:F:109:ASP:OD2	1:F:109:ASP:O	2.39	0.41
1:A:131:THR:HG21	1:A:137:PHE:HE2	1.86	0.41
1:A:194:ARG:HA	1:A:194:ARG:HD3	1.77	0.41
1:F:153:LEU:HD23	1:F:236:ILE:HG21	1.96	0.41
1:C:101:PRO:O	1:C:105:ARG:CD	2.51	0.41
1:E:118:VAL:HG12	1:E:119:GLN:H	1.83	0.41
1:F:222:THR:HB	1:F:237:THR:CB	2.50	0.41
1:A:78:GLU:OE2	1:A:81:LEU:HD23	2.20	0.41
1:F:152:SER:N	1:F:172:THR:O	2.52	0.41
1:D:94:TYR:HB3	1:D:98:VAL:HG23	2.03	0.41
1:F:165:LEU:HA	1:F:210:LEU:O	2.21	0.41
1:D:213:SER:O	1:D:242:VAL:HG11	2.21	0.41
1:D:197:LYS:HZ3	1:D:202:ALA:HB2	1.86	0.41
1:E:149:PRO:HG2	1:E:234:GLN:HE21	1.84	0.41
1:C:178:ALA:HB2	1:C:202:ALA:HB3	2.02	0.41
1:A:35:GLU:OE2	1:A:55:ARG:CD	2.69	0.41
1:A:227:HIS:CD2	1:A:228:PRO:HD2	2.56	0.40
1:B:116:ASN:N	1:B:116:ASN:HD22	2.18	0.40
1:C:118:VAL:CG1	1:C:119:GLN:N	2.85	0.40
1:D:194:ARG:NH2	1:E:150:LEU:HG	2.36	0.40
1:D:224:VAL:CG2	1:D:224:VAL:O	2.70	0.40
1:E:90:VAL:HG21	1:E:94:TYR:C	2.41	0.40
1:A:183:TRP:CD1	1:A:191:THR:HG21	2.57	0.40
1:E:60:GLU:HG2	1:E:133:PRO:HD2	2.04	0.40
1:C:70:VAL:HG21	1:C:124:GLU:HB3	2.01	0.40
1:B:34:LEU:HD21	1:B:52:CYS:SG	2.61	0.40
1:E:184:ASP:O	1:E:222:THR:HG23	2.21	0.40
1:A:122:GLU:OE2	1:A:144:ARG:NH1	2.43	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	213/218 (98%)	206 (97%)	7 (3%)	0	100	100
1	B	211/218 (97%)	204 (97%)	7 (3%)	0	100	100
1	C	209/218 (96%)	199 (95%)	10 (5%)	0	100	100
1	D	210/218 (96%)	197 (94%)	12 (6%)	1 (0%)	34	78
1	E	206/218 (94%)	190 (92%)	16 (8%)	0	100	100
1	F	181/218 (83%)	167 (92%)	14 (8%)	0	100	100
All	All	1230/1308 (94%)	1163 (95%)	66 (5%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	59	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	176/181 (97%)	160 (91%)	16 (9%)	12	46
1	B	176/181 (97%)	145 (82%)	31 (18%)	2	13
1	C	171/181 (94%)	146 (85%)	25 (15%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	169/181 (93%)	142 (84%)	27 (16%)	3	18
1	E	165/181 (91%)	143 (87%)	22 (13%)	5	26
1	F	150/181 (83%)	120 (80%)	30 (20%)	1	9
All	All	1007/1086 (93%)	856 (85%)	151 (15%)	3	21

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ASP
1	A	114	LEU
1	A	131	THR
1	A	143	LEU
1	A	147	VAL
1	A	152	SER
1	A	161	GLU
1	A	192	SER
1	A	200	ARG
1	A	205	THR
1	A	210	LEU
1	A	222	THR
1	A	225	VAL
1	A	242	VAL
1	A	243	SER
1	A	244	HIS
1	B	33	GLU
1	B	34	LEU
1	B	41	THR
1	B	55	ARG
1	B	58	SER
1	B	61	GLN
1	B	71	ASP
1	B	85	LYS
1	B	97	ARG
1	B	98	VAL
1	B	105	ARG
1	B	114	LEU
1	B	116	ASN
1	B	131	THR
1	B	140	ARG
1	B	144	ARG
1	B	147	VAL

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Mol	Chain	Res	Type
1	B	152	SER
1	B	161	GLU
1	B	188	LYS
1	B	192	SER
1	B	197	LYS
1	B	200	ARG
1	B	205	THR
1	B	210	LEU
1	B	217	ASN
1	B	222	THR
1	B	224	VAL
1	B	225	VAL
1	B	231	LEU
1	B	244	HIS
1	C	49	LYS
1	C	62	VAL
1	C	70	VAL
1	C	71	ASP
1	C	95	GLU
1	C	97	ARG
1	C	106	ASN
1	C	108	LEU
1	C	113	LEU
1	C	129	VAL
1	C	130	SER
1	C	131	THR
1	C	147	VAL
1	C	152	SER
1	C	153	LEU
1	C	192	SER
1	C	193	SER
1	C	199	SER
1	C	205	THR
1	C	210	LEU
1	C	213	SER
1	C	217	ASN
1	C	222	THR
1	C	224	VAL
1	C	225	VAL
1	D	38	ASP
1	D	42	VAL
1	D	46	GLN

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Mol	Chain	Res	Type
1	D	58	SER
1	D	69	ARG
1	D	70	VAL
1	D	71	ASP
1	D	78	GLU
1	D	79	LEU
1	D	114	LEU
1	D	121	ASP
1	D	124	GLU
1	D	131	THR
1	D	138	GLN
1	D	142	ARG
1	D	146	LEU
1	D	147	VAL
1	D	154	ASN
1	D	161	GLU
1	D	172	THR
1	D	190	THR
1	D	197	LYS
1	D	210	LEU
1	D	214	ARG
1	D	215	SER
1	D	219	GLN
1	D	222	THR
1	E	41	THR
1	E	42	VAL
1	E	60	GLU
1	E	62	VAL
1	E	70	VAL
1	E	100	GLN
1	E	114	LEU
1	E	138	GLN
1	E	140	ARG
1	E	143	LEU
1	E	147	VAL
1	E	152	SER
1	E	182	THR
1	E	197	LYS
1	E	200	ARG
1	E	201	SER
1	E	205	THR
1	E	210	LEU

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Mol	Chain	Res	Type
1	E	222	THR
1	E	225	VAL
1	E	230	LEU
1	E	239	ILE
1	F	44	LEU
1	F	70	VAL
1	F	109	ASP
1	F	111	SER
1	F	112	VAL
1	F	113	LEU
1	F	114	LEU
1	F	118	VAL
1	F	129	VAL
1	F	131	THR
1	F	140	ARG
1	F	152	SER
1	F	153	LEU
1	F	159	LEU
1	F	160	GLU
1	F	165	LEU
1	F	166	THR
1	F	170	SER
1	F	171	CYS
1	F	184	ASP
1	F	191	THR
1	F	194	ARG
1	F	204	VAL
1	F	205	THR
1	F	214	ARG
1	F	222	THR
1	F	224	VAL
1	F	225	VAL
1	F	231	LEU
1	F	234	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	GLN
1	B	116	ASN
1	B	217	ASN
1	B	219	GLN

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Mol	Chain	Res	Type
1	C	119	GLN
1	C	163	GLN
1	C	217	ASN
1	D	100	GLN
1	D	219	GLN
1	D	244	HIS
1	E	46	GLN
1	E	61	GLN
1	E	64	GLN
1	E	198	HIS
1	E	232	GLN
1	E	234	GLN
1	F	77	GLN
1	F	198	HIS
1	F	234	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 carbohydrates 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, 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	215/218 (98%)	-0.40	0 100 100	35, 59, 99, 131	0
1	B	213/218 (97%)	-0.39	1 (0%) 91 88	40, 58, 89, 133	0
1	C	211/218 (96%)	-0.31	1 (0%) 91 88	39, 58, 121, 148	0
1	D	212/218 (97%)	-0.06	8 (3%) 44 36	68, 107, 148, 189	0
1	E	208/218 (95%)	0.26	19 (9%) 11 10	55, 118, 206, 260	0
1	F	189/218 (86%)	0.56	19 (10%) 9 9	114, 145, 192, 263	0
All	All	1248/1308 (95%)	-0.07	48 (3%) 44 36	35, 84, 168, 263	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	107	PRO	5.4
1	E	87	GLY	4.7
1	E	86	TYR	4.6
1	E	56	GLY	4.2
1	E	133	PRO	3.9
1	D	37	SER	3.9
1	E	102	PRO	3.7
1	F	142	ARG	3.6
1	E	61	GLN	3.5
1	E	72	ALA	3.1
1	E	104	PRO	3.0
1	E	83	HIS	3.0
1	E	76	ALA	2.9
1	E	75	GLY	2.9
1	F	39	VAL	2.8
1	E	164	GLY	2.8
1	F	76	ALA	2.7
1	F	163	GLN	2.7
1	F	103	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	106	ASN	2.6
1	E	60	GLU	2.6
1	F	71	ASP	2.6
1	C	160	GLU	2.6
1	D	72	ALA	2.6
1	F	75	GLY	2.6
1	F	160	GLU	2.6
1	E	163	GLN	2.5
1	E	71	ASP	2.5
1	E	73	GLY	2.5
1	D	71	ASP	2.5
1	E	58	SER	2.5
1	F	162	GLY	2.5
1	F	104	PRO	2.4
1	B	73	GLY	2.4
1	D	73	GLY	2.4
1	E	74	GLU	2.4
1	F	73	GLY	2.3
1	F	184	ASP	2.3
1	E	88	LEU	2.3
1	F	38	ASP	2.3
1	D	104	PRO	2.2
1	D	75	GLY	2.2
1	D	92	PRO	2.2
1	F	72	ALA	2.2
1	F	190	THR	2.2
1	D	76	ALA	2.1
1	F	161	GLU	2.1
1	F	246	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.