



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2025 – 04:31 PM JST

PDB ID : 7FCA
Title : PfkB(Mycobacterium marinum)
Authors : Li, J.; Gao, B.; Ji, R.
Deposited on : 2021-07-14
Resolution : 2.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

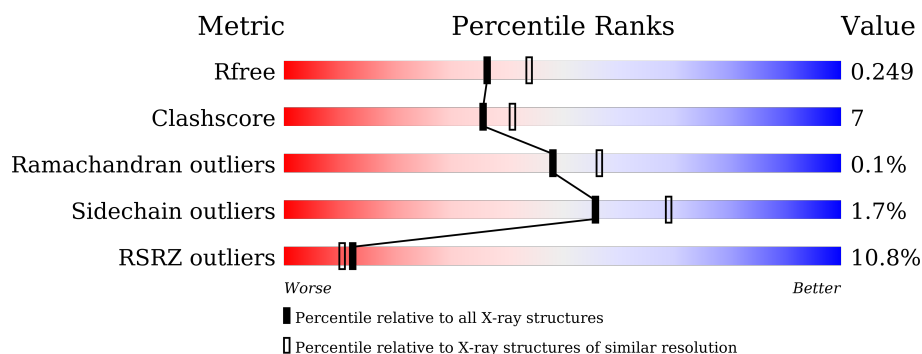
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (2.24-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	303	<div> <div>7%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	B	303	<div> <div>14%</div> <div>72%</div> <div>17%</div> <div>10%</div> </div>
1	C	303	<div> <div>8%</div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
1	E	303	<div> <div>7%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
1	F	303	<div> <div>15%</div> <div>73%</div> <div>16%</div> <div>11%</div> </div>
2	D	291	<div> <div>9%</div> <div>88%</div> <div>8%</div> <div></div> </div>

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
3	GOL	B	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11955 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 Fructokinase, PfkB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			1991	1253	355	378	5			
1	B	272	Total	C	N	O	S	0	0	0
			1937	1218	341	374	4			
1	C	273	Total	C	N	O	S	0	0	0
			1929	1212	344	369	4			
1	E	278	Total	C	N	O	S	0	0	0
			1966	1236	349	377	4			
1	F	270	Total	C	N	O	S	0	0	0
			1905	1200	341	360	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	THR	ALA	conflict	UNP B2HEF4
B	108	THR	ALA	conflict	UNP B2HEF4
C	108	THR	ALA	conflict	UNP B2HEF4
E	108	THR	ALA	conflict	UNP B2HEF4
F	108	THR	ALA	conflict	UNP B2HEF4

- Molecule 2 is a protein called Fructokinase, PfkB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	282	Total	C	N	O	S	0	0	0
			2011	1264	359	384	4			

There is a discrepancy between the modelled and reference sequences:

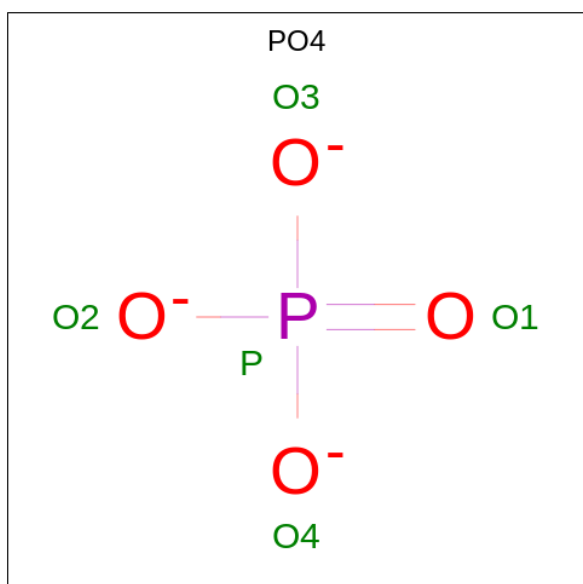
Chain	Residue	Modelled	Actual	Comment	Reference
D	161	ARG	GLU	conflict	UNP B2HEF4

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

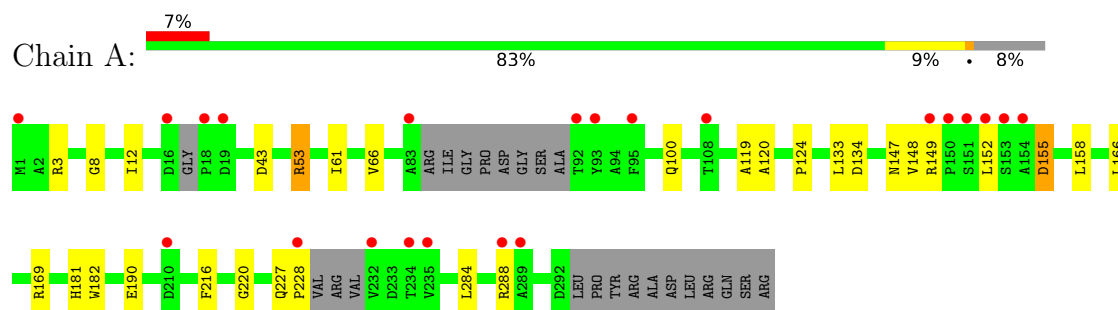
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	49	Total O 49 49	0	0
5	B	23	Total O 23 23	0	0
5	C	17	Total O 17 17	0	0
5	D	40	Total O 40 40	0	0
5	E	18	Total O 18 18	0	0
5	F	14	Total O 14 14	0	0

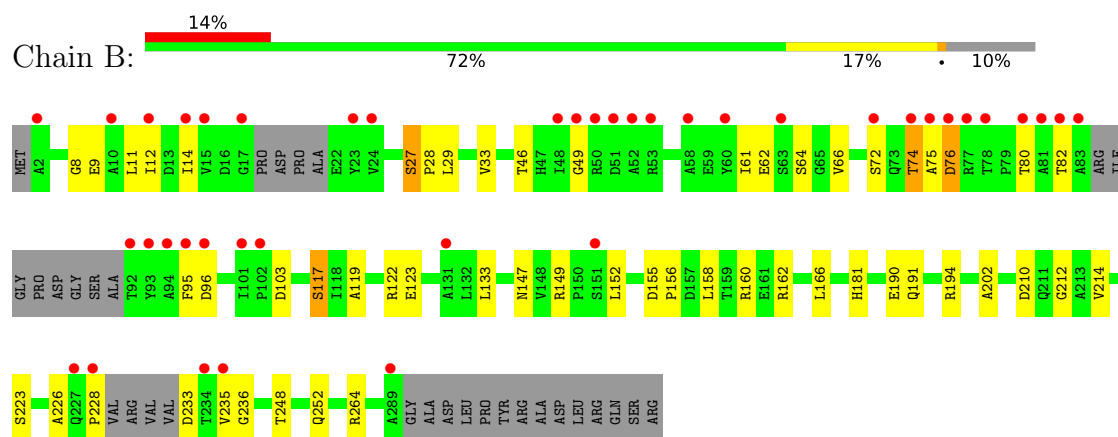
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

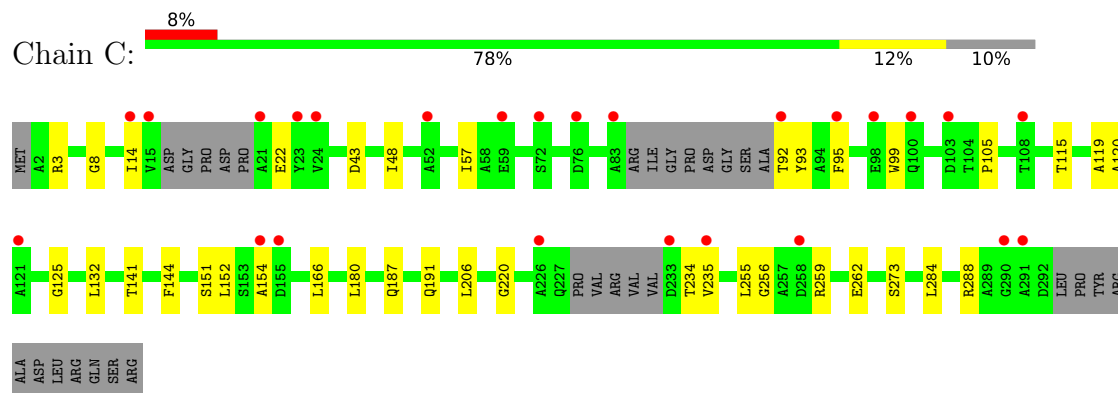
• Molecule 1: Fructokinase, PfkB



• Molecule 1: Fructokinase, PfkB



• Molecule 1: Fructokinase, PfkB



Chain E:

7%

82%

9%

8%

Chain F:

15% 73% 16% 11%

VAL VAL D233 D234 V235 G236 M242 T248 Q252 S282 A289 G290 ALA ASP LEU PRO TYR ARG ALA ASP LEU ARG GLN SER ARG

SER THR Y93 A94 F95 D96 L97 Q100 T101 P102 D103 T104 P105 P106 V107 T108 A119 A120 A121 R122 E123 P124 G125 A130 A131 L132 P146 R149 P150 S151 L152 S153 L158 T159 R160 L166 R169 K174 D179 I183 D184 D185 A186 R187 R188 R189 R190 R191 R192 R193 R194 R195 R196 R197 R198 R199 R200 R201 R202 R203 R204 R205 R206 R207 R208 R209 R210 R211 R212 R213 R214 R215 R216 R217 R218 R219 R220 R221 R222 R223 R224 R225 R226 R227 R228 R229 R230 R231 R232 R233 R234 R235 R236 R237 R238 R239 R240 R241 R242 R243 R244 R245 R246 R247 R248 R249 R250 R251 R252 R253 R254 R255 R256 R257 R258 R259 R260 R261 R262 R263 R264 R265 R266 R267 R268 R269 R270 R271 R272 R273 R274 R275 R276 R277 R278 R279 R280 R281 R282 R283 R284 R285 R286 R287 R288 R289 R290 R291 R292 R293 R294 R295 R296 R297 R298 R299 R300 R301 R302 R303 R304 R305 R306 R307 R308 R309 R310 R311 R312 R313 R314 R315 R316 R317 R318 R319 R320 R321 R322 R323 R324 R325 R326 R327 R328 R329 R330 R331 R332 R333 R334 R335 R336 R337 R338 R339 R340 R341 R342 R343 R344 R345 R346 R347 R348 R349 R350 R351 R352 R353 R354 R355 R356 R357 R358 R359 R360 R361 R362 R363 R364 R365 R366 R367 R368 R369 R370 R371 R372 R373 R374 R375 R376 R377 R378 R379 R380 R381 R382 R383 R384 R385 R386 R387 R388 R389 R390 R391 R392 R393 R394 R395 R396 R397 R398 R399 R400 R401 R402 R403 R404 R405 R406 R407 R408 R409 R410 R411 R412 R413 R414 R415 R416 R417 R418 R419 R420 R421 R422 R423 R424 R425 R426 R427 R428 R429 R430 R431 R432 R433 R434 R435 R436 R437 R438 R439 R440 R441 R442 R443 R444 R445 R446 R447 R448 R449 R450 R451 R452 R453 R454 R455 R456 R457 R458 R459 R460 R461 R462 R463 R464 R465 R466 R467 R468 R469 R470 R471 R472 R473 R474 R475 R476 R477 R478 R479 R480 R481 R482 R483 R484 R485 R486 R487 R488 R489 R490 R491 R492 R493 R494 R495 R496 R497 R498 R499 R500 R501 R502 R503 R504 R505 R506 R507 R508 R509 R510 R511 R512 R513 R514 R515 R516 R517 R518 R519 R520 R521 R522 R523 R524 R525 R526 R527 R528 R529 R530 R531 R532 R533 R534 R535 R536 R537 R538 R539 R540 R541 R542 R543 R544 R545 R546 R547 R548 R549 R550 R551 R552 R553 R554 R555 R556 R557 R558 R559 R560 R561 R562 R563 R564 R565 R566 R567 R568 R569 R570 R571 R572 R573 R574 R575 R576 R577 R578 R579 R580 R581 R582 R583 R584 R585 R586 R587 R588 R589 R590 R591 R592 R593 R594 R595 R596 R597 R598 R599 R600 R601 R602 R603 R604 R605 R606 R607 R608 R609 R610 R611 R612 R613 R614 R615 R616 R617 R618 R619 R620 R621 R622 R623 R624 R625 R626 R627 R628 R629 R630 R631 R632 R633 R634 R635 R636 R637 R638 R639 R640 R641 R642 R643 R644 R645 R646 R647 R648 R649 R650 R651 R652 R653 R654 R655 R656 R657 R658 R659 R660 R661 R662 R663 R664 R665 R666 R667 R668 R669 R670 R671 R672 R673 R674 R675 R676 R677 R678 R679 R680 R681 R682 R683 R684 R685 R686 R687 R688 R689 R690 R691 R692 R693 R694 R695 R696 R697 R698 R699 R700 R701 R702 R703 R704 R705 R706 R707 R708 R709 R710 R711 R712 R713 R714 R715 R716 R717 R718 R719 R720 R721 R722 R723 R724 R725 R726 R727 R728 R729 R730 R731 R732 R733 R734 R735 R736 R737 R738 R739 R740 R741 R742 R743 R744 R745 R746 R747 R748 R749 R750 R751 R752 R753 R754 R755 R756 R757 R758 R759 R760 R761 R762 R763 R764 R765 R766 R767 R768 R769 R770 R771 R772 R773 R774 R775 R776 R777 R778 R779 R780 R781 R782 R783 R784 R785 R786 R787 R788 R789 R790 R791 R792 R793 R794 R795 R796 R797 R798 R799 R800 R801 R802 R803 R804 R805 R806 R807 R808 R809 R810 R811 R812 R813 R814 R815 R816 R817 R818 R819 R820 R821 R822 R823 R824 R825 R826 R827 R828 R829 R830 R831 R832 R833 R834 R835 R836 R837 R838 R839 R840 R841 R842 R843 R844 R845 R846 R847 R848 R849 R850 R851 R852 R853 R854 R855 R856 R857 R858 R859 R860 R861 R862 R863 R864 R865 R866 R867 R868 R869 R870 R871 R872 R873 R874 R875 R876 R877 R878 R879 R880 R881 R882 R883 R884 R885 R886 R887 R888 R889 R890 R891 R892 R893 R894 R895 R896 R897 R898 R899 R900 R901 R902 R903 R904 R905 R906 R907 R908 R909 R910 R911 R912 R913 R914 R915 R916 R917 R918 R919 R920 R921 R922 R923 R924 R925 R926 R927 R928 R929 R930 R931 R932 R933 R934 R935 R936 R937 R938 R939 R940 R941 R942 R943 R944 R945 R946 R947 R948 R949 R950 R951 R952 R953 R954 R955 R956 R957 R958 R959 R960 R961 R962 R963 R964 R965 R966 R967 R968 R969 R970 R971 R972 R973 R974 R975 R976 R977 R978 R979 R980 R981 R982 R983 R984 R985 R986 R987 R988 R989 R990 R991 R992 R993 R994 R995 R996 R997 R998 R999

Chain D:

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.41Å 125.41Å 137.52Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	66.92 – 2.21 66.92 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.8 (66.92-2.21) 99.8 (66.92-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.212 , 0.245 0.215 , 0.249	Depositor DCC
R_{free} test set	5115 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11955	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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 39.62 % 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 3.0880e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4

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	0.52	0/2025	0.64	0/2774
1	B	0.52	0/1969	0.65	1/2699 (0.0%)
1	C	0.39	0/1960	0.56	0/2686
1	E	0.39	0/1999	0.57	0/2742
1	F	0.43	0/1935	0.59	0/2652
2	D	0.48	0/2046	0.62	1/2805 (0.0%)
All	All	0.46	0/11934	0.61	2/16358 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	102	PRO	N-CA-CB	5.84	110.31	103.30
1	B	228	PRO	N-CA-CB	5.67	110.11	103.30

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	1991	0	1969	31	0
1	B	1937	0	1888	43	0
1	C	1929	0	1900	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1966	0	1935	23	0
1	F	1905	0	1878	39	0
2	D	2011	0	1993	19	0
3	A	6	0	8	1	0
3	B	12	0	16	5	0
3	D	6	0	8	2	0
3	E	6	0	8	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	49	0	0	1	0
5	B	23	0	0	1	0
5	C	17	0	0	0	0
5	D	40	0	0	1	0
5	E	18	0	0	1	0
5	F	14	0	0	0	0
All	All	11955	0	11603	168	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 7.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASP:OD2	1:B:236:GLY:HA3	1.38	1.19
1:A:284:LEU:HD21	1:A:288:ARG:NH1	1.66	1.09
1:A:284:LEU:HD21	1:A:288:ARG:HH11	1.18	1.00
1:F:160:ARG:HG3	1:F:160:ARG:HH11	1.39	0.88
1:B:12:ILE:CD1	3:B:401:GOL:H12	2.04	0.87
1:E:12:ILE:HD13	1:E:53:ARG:HB3	1.59	0.84
1:B:12:ILE:HD11	3:B:401:GOL:H12	1.59	0.83
1:E:12:ILE:CD1	1:E:53:ARG:HB3	2.11	0.81
1:B:149:ARG:NH1	1:B:235:VAL:HG21	1.97	0.78
1:B:235:VAL:HG12	5:B:521:HOH:O	1.84	0.78
1:F:47:HIS:HD2	1:F:100:GLN:H	1.28	0.78
1:B:12:ILE:HD13	3:B:401:GOL:H32	1.68	0.75
1:E:12:ILE:HD13	1:E:53:ARG:HD2	1.69	0.75
1:B:76:ASP:OD1	1:B:76:ASP:N	2.09	0.74
1:F:48:ILE:HD11	1:F:57:ILE:HB	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:CD2	1:A:288:ARG:HH11	2.01	0.72
1:F:76:ASP:OD1	1:F:76:ASP:N	2.18	0.70
1:F:160:ARG:HG3	1:F:160:ARG:NH1	2.04	0.69
1:F:122:ARG:HD2	1:F:152:LEU:HD11	1.74	0.69
1:A:155:ASP:HB3	2:D:161:ARG:HG2	1.74	0.68
1:F:149:ARG:NH2	1:F:235:VAL:HG11	2.08	0.68
1:F:149:ARG:HH22	1:F:235:VAL:HG11	1.60	0.66
1:F:152:LEU:HD23	1:F:152:LEU:O	1.96	0.66
1:C:14:ILE:HG23	1:C:22:GLU:HG2	1.79	0.65
2:D:264:ARG:HH12	3:D:301:GOL:H11	1.62	0.65
1:A:149:ARG:O	1:A:152:LEU:HB3	1.97	0.65
1:B:12:ILE:CD1	3:B:401:GOL:H32	2.26	0.65
1:B:12:ILE:HD13	3:B:401:GOL:H12	1.79	0.65
1:B:133:LEU:HD12	1:B:166:LEU:HD22	1.80	0.62
1:A:12:ILE:HG13	1:A:53:ARG:HB3	1.81	0.62
1:A:181:HIS:CD2	1:C:220:GLY:HA2	2.35	0.62
1:F:80:THR:OG1	1:F:96:ASP:HB3	2.00	0.61
1:F:14:ILE:HB	1:F:82:THR:HA	1.83	0.60
1:B:46:THR:H	1:B:72:SER:HB2	1.67	0.60
1:C:3:ARG:NH1	1:C:43:ASP:OD1	2.36	0.59
1:E:179:ASP:O	1:E:183:ILE:HG12	2.02	0.59
1:B:80:THR:HG22	1:B:96:ASP:HB3	1.84	0.58
1:A:155:ASP:OD2	1:A:155:ASP:N	2.31	0.58
1:A:227:GLN:OE1	1:A:228:PRO:HD2	2.04	0.58
1:B:61:ILE:HG23	1:B:66:VAL:HB	1.84	0.58
1:B:27:SER:OG	1:B:147:ASN:ND2	2.36	0.57
1:F:47:HIS:HD2	1:F:100:GLN:N	2.02	0.57
1:A:155:ASP:CB	2:D:161:ARG:HG2	2.36	0.56
1:B:62:GLU:OE2	1:B:62:GLU:HA	2.07	0.55
2:D:181:HIS:CD2	1:E:220:GLY:HA2	2.43	0.54
1:F:11:LEU:HD21	1:F:97:LEU:HD12	1.90	0.54
1:A:147:ASN:OD1	3:A:401:GOL:O1	2.26	0.54
1:C:180:LEU:HD22	1:C:206:LEU:HD13	1.90	0.54
1:B:149:ARG:HH12	1:B:235:VAL:HG11	1.72	0.54
1:C:48:ILE:HG21	1:C:57:ILE:HG21	1.89	0.54
1:A:149:ARG:O	1:A:152:LEU:N	2.41	0.53
1:B:190:GLU:O	1:B:194:ARG:HG3	2.08	0.53
1:E:181:HIS:CE1	1:F:220:GLY:HA2	2.45	0.52
1:E:8:GLY:HA2	1:E:119:ALA:CB	2.40	0.52
1:C:120:ALA:HB1	1:C:166:LEU:HD12	1.91	0.52
2:D:174:LYS:NZ	5:D:403:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:GLY:HA2	1:E:119:ALA:HB2	1.91	0.51
1:B:122:ARG:HD3	1:B:152:LEU:HD21	1.92	0.51
1:A:100:GLN:HE21	1:A:124:PRO:HG2	1.74	0.51
1:C:95:PHE:CB	1:C:152:LEU:HD23	2.41	0.51
1:B:155:ASP:HB3	1:B:158:LEU:HB2	1.93	0.50
1:A:61:ILE:HG23	1:A:66:VAL:HB	1.92	0.50
1:E:145:ASP:HB2	1:E:242:MET:HE2	1.93	0.50
1:B:29:LEU:C	1:B:29:LEU:HD23	2.32	0.50
1:B:27:SER:HB3	1:B:28:PRO:HD3	1.94	0.49
1:E:259:ARG:NH2	1:E:262:GLU:HG2	2.28	0.49
1:F:152:LEU:HD23	1:F:152:LEU:C	2.32	0.49
1:F:47:HIS:CE1	1:F:74:THR:HG23	2.48	0.48
1:A:220:GLY:HA2	1:B:181:HIS:CD2	2.48	0.48
1:A:158:LEU:HD13	2:D:159:THR:HG21	1.94	0.48
2:D:99:TRP:CZ2	2:D:119:ALA:HB1	2.49	0.48
2:D:264:ARG:HH22	3:D:301:GOL:H2	1.78	0.48
1:F:105:PRO:HB2	1:F:107:VAL:HG23	1.95	0.48
1:B:149:ARG:HH11	1:B:235:VAL:HG21	1.78	0.48
1:F:48:ILE:O	1:F:75:ALA:HB3	2.14	0.48
1:F:79:PRO:HB3	1:F:97:LEU:CB	2.43	0.48
1:C:92:THR:C	1:C:93:TYR:HD2	2.17	0.47
1:B:14:ILE:CB	1:B:82:THR:HG22	2.44	0.47
1:C:8:GLY:HA2	1:C:119:ALA:CB	2.43	0.47
1:F:24:VAL:HG11	1:F:60:TYR:CD2	2.49	0.47
1:A:149:ARG:O	1:A:152:LEU:CB	2.61	0.47
1:F:54:GLY:CA	1:F:78:THR:HG21	2.45	0.47
1:E:3:ARG:NH1	1:E:41:ASP:HB3	2.30	0.47
2:D:107:VAL:HG12	2:D:108:ALA:O	2.15	0.47
1:F:107:VAL:HG12	1:F:108:THR:O	2.15	0.47
1:A:190:GLU:HG3	1:A:216:PHE:CZ	2.50	0.47
1:F:12:ILE:HD12	1:F:23:TYR:O	2.15	0.47
1:B:9:GLU:O	1:B:9:GLU:HG2	2.14	0.46
1:C:141:THR:HG23	1:C:256:GLY:N	2.31	0.46
2:D:152:LEU:HD11	2:D:182:TRP:CD1	2.51	0.46
1:E:8:GLY:HA3	1:E:28:PRO:HG2	1.96	0.46
1:B:8:GLY:HA3	1:B:28:PRO:HG2	1.97	0.46
1:B:191:GLN:NE2	1:C:191:GLN:HE21	2.14	0.46
1:E:51:ASP:N	1:E:51:ASP:OD1	2.50	0.45
1:B:123:GLU:OE2	1:B:162:ARG:NH1	2.33	0.45
1:E:43:ASP:HB3	1:E:69:VAL:CG2	2.46	0.45
1:F:59:GLU:O	1:F:63:SER:OG	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:CD2	1:B:152:LEU:HB2	2.52	0.45
1:B:49:GLY:N	1:B:75:ALA:HB3	2.31	0.45
1:F:12:ILE:HG22	1:F:80:THR:HA	1.99	0.45
1:A:155:ASP:OD1	2:D:161:ARG:HG2	2.16	0.45
1:B:214:VAL:HG12	1:B:223:SER:HB3	1.99	0.45
1:C:141:THR:HG21	1:C:255:LEU:HA	1.99	0.45
2:D:262:GLU:OE1	2:D:262:GLU:N	2.46	0.45
1:C:187:GLN:NE2	1:C:191:GLN:HG2	2.31	0.44
1:F:12:ILE:CG2	1:F:80:THR:HG22	2.47	0.44
1:B:74:THR:O	1:B:74:THR:OG1	2.35	0.44
1:E:74:THR:HG22	1:E:74:THR:O	2.16	0.44
1:E:14:ILE:HD12	1:E:82:THR:HG22	1.99	0.44
1:F:160:ARG:NH1	1:F:160:ARG:CG	2.76	0.44
1:C:259:ARG:HA	1:C:262:GLU:OE2	2.18	0.44
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.79	0.44
2:D:259:ARG:HH21	2:D:262:GLU:HG2	1.83	0.44
1:F:169:ARG:HH21	1:F:169:ARG:HG3	1.83	0.44
1:B:11:LEU:HD12	1:B:11:LEU:C	2.38	0.44
1:B:27:SER:CB	1:B:28:PRO:HD3	2.47	0.44
2:D:214:VAL:HG12	2:D:223:SER:HB3	2.00	0.43
1:F:79:PRO:HB3	1:F:97:LEU:HA	1.99	0.43
1:A:3:ARG:NH1	1:A:43:ASP:OD1	2.51	0.43
1:E:174:LYS:NZ	5:E:503:HOH:O	2.40	0.43
1:A:8:GLY:HA2	1:A:119:ALA:CB	2.48	0.43
1:A:133:LEU:HD12	1:A:166:LEU:HD22	2.01	0.43
1:C:93:TYR:O	1:C:151:SER:HB3	2.18	0.43
1:F:54:GLY:N	1:F:78:THR:HG21	2.33	0.43
1:F:61:ILE:HG23	1:F:66:VAL:HB	1.99	0.43
1:B:156:PRO:HB2	1:B:160:ARG:HH12	1.83	0.43
1:A:148:VAL:HG23	1:A:148:VAL:O	2.18	0.43
2:D:149:ARG:N	2:D:150:PRO:HD2	2.33	0.43
1:B:212:GLY:N	1:B:226:ALA:HB2	2.34	0.43
2:D:120:ALA:HB1	2:D:166:LEU:HD12	2.01	0.43
1:B:33:VAL:HG13	1:B:64:SER:CB	2.49	0.43
2:D:5:LEU:O	2:D:113:VAL:HA	2.19	0.43
1:B:191:GLN:NE2	1:C:187:GLN:OE1	2.51	0.43
1:A:100:GLN:NE2	1:A:124:PRO:HG2	2.34	0.42
1:A:149:ARG:O	1:A:152:LEU:HD23	2.19	0.42
1:A:152:LEU:HD13	1:A:182:TRP:CZ2	2.54	0.42
1:C:8:GLY:HA2	1:C:119:ALA:HB2	2.01	0.42
1:F:179:ASP:O	1:F:183:ILE:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLY:HA2	1:A:119:ALA:HB2	2.01	0.42
1:E:207:THR:HB	3:E:401:GOL:H31	2.01	0.42
1:F:248:THR:O	1:F:252:GLN:HG3	2.19	0.42
1:B:9:GLU:OE1	1:B:117:SER:HB3	2.20	0.42
1:E:15:VAL:HG12	1:E:16:ASP:N	2.35	0.42
1:A:120:ALA:HB1	1:A:166:LEU:HD12	2.02	0.41
1:A:134:ASP:OD2	1:A:169:ARG:NH2	2.53	0.41
2:D:120:ALA:HB1	2:D:166:LEU:CD1	2.50	0.41
1:F:146:PRO:HD2	1:F:174:LYS:O	2.20	0.41
1:A:100:GLN:NE2	1:A:100:GLN:HA	2.35	0.41
1:C:105:PRO:HA	1:C:132:LEU:HD21	2.01	0.41
1:F:79:PRO:HB3	1:F:97:LEU:HB2	2.02	0.41
1:A:53:ARG:HG3	5:A:535:HOH:O	2.19	0.41
1:B:8:GLY:HA2	1:B:119:ALA:HB2	2.02	0.41
1:E:14:ILE:HB	1:E:82:THR:HG22	2.01	0.41
1:E:61:ILE:HG23	1:E:66:VAL:HB	2.03	0.41
1:F:8:GLY:HA3	1:F:28:PRO:HG2	2.02	0.41
1:F:169:ARG:HH21	1:F:169:ARG:CG	2.34	0.41
1:E:149:ARG:HD3	1:E:149:ARG:HA	1.89	0.41
1:B:191:GLN:HE21	1:C:191:GLN:HE21	1.67	0.41
1:B:248:THR:O	1:B:252:GLN:HG3	2.20	0.41
1:E:48:ILE:O	1:E:73:GLN:HA	2.21	0.41
1:F:8:GLY:HA2	1:F:119:ALA:CB	2.51	0.41
1:B:202:ALA:HB1	1:B:264:ARG:HA	2.01	0.41
1:C:284:LEU:HG	1:C:288:ARG:HD2	2.02	0.41
1:C:115:THR:O	1:C:144:PHE:HA	2.21	0.41
1:F:120:ALA:HB1	1:F:166:LEU:HD12	2.04	0.40
1:C:99:TRP:CD1	1:C:125:GLY:HA3	2.56	0.40
1:C:234:THR:HG22	1:C:235:VAL:H	1.86	0.40
2:D:79:PRO:HA	2:D:96:ASP:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	272/303 (90%)	267 (98%)	5 (2%)	0	100	100
1	B	264/303 (87%)	257 (97%)	7 (3%)	0	100	100
1	C	265/303 (88%)	253 (96%)	11 (4%)	1 (0%)	30	33
1	E	270/303 (89%)	265 (98%)	5 (2%)	0	100	100
1	F	260/303 (86%)	254 (98%)	6 (2%)	0	100	100
2	D	276/291 (95%)	270 (98%)	6 (2%)	0	100	100
All	All	1607/1806 (89%)	1566 (97%)	40 (2%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	154	ALA

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	193/228 (85%)	191 (99%)	2 (1%)	73	83
1	B	186/228 (82%)	180 (97%)	6 (3%)	34	43
1	C	186/228 (82%)	185 (100%)	1 (0%)	86	93
1	E	190/228 (83%)	188 (99%)	2 (1%)	70	81
1	F	182/228 (80%)	176 (97%)	6 (3%)	33	42
2	D	196/216 (91%)	194 (99%)	2 (1%)	73	83
All	All	1133/1356 (84%)	1114 (98%)	19 (2%)	56	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG

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Mol	Chain	Res	Type
1	A	155	ASP
1	B	27	SER
1	B	74	THR
1	B	76	ASP
1	B	103	ASP
1	B	117	SER
1	B	210	ASP
1	C	273	SER
2	D	174	LYS
2	D	232	VAL
1	E	73	GLN
1	E	174	LYS
1	F	76	ASP
1	F	103	ASP
1	F	151	SER
1	F	158	LEU
1	F	166	LEU
1	F	242	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	C	191	GLN
1	F	47	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	A	402	-	4,4,4	0.80	0	6,6,6	0.76	0
3	GOL	A	401	-	5,5,5	1.22	0	5,5,5	0.95	0
4	PO4	E	402	-	4,4,4	0.81	0	6,6,6	0.52	0
4	PO4	F	401	-	4,4,4	0.81	0	6,6,6	0.43	0
3	GOL	B	402	-	5,5,5	0.75	0	5,5,5	1.14	0
3	GOL	D	301	-	5,5,5	0.90	0	5,5,5	1.00	0
3	GOL	B	401	-	5,5,5	0.88	0	5,5,5	1.08	0
4	PO4	D	302	-	4,4,4	0.84	0	6,6,6	0.45	0
3	GOL	E	401	-	5,5,5	0.95	0	5,5,5	0.96	0
4	PO4	B	403	-	4,4,4	0.81	0	6,6,6	0.58	0

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	GOL	A	401	-	-	2/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	D	301	-	-	2/4/4/4	-
3	GOL	B	401	-	-	1/4/4/4	-
3	GOL	E	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	C1-C2-C3-O3
3	E	401	GOL	O1-C1-C2-C3
3	A	401	GOL	O2-C2-C3-O3
3	D	301	GOL	C1-C2-C3-O3
3	E	401	GOL	O1-C1-C2-O2
3	D	301	GOL	O2-C2-C3-O3
3	B	401	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GOL	1	0
3	D	301	GOL	2	0
3	B	401	GOL	5	0
3	E	401	GOL	1	0

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	280/303 (92%)	0.36	22 (7%)	20 18	34, 48, 83, 99	0
1	B	272/303 (89%)	0.84	41 (15%)	6 5	43, 59, 90, 101	0
1	C	273/303 (90%)	0.80	25 (9%)	16 14	44, 65, 91, 105	0
1	E	278/303 (91%)	0.62	20 (7%)	23 21	46, 60, 86, 105	0
1	F	270/303 (89%)	1.03	44 (16%)	5 4	42, 62, 97, 104	0
2	D	282/291 (96%)	0.44	26 (9%)	16 14	36, 52, 78, 108	0
All	All	1655/1806 (91%)	0.68	178 (10%)	12 10	34, 58, 91, 108	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	ARG	7.7
1	F	235	VAL	7.5
2	D	1	MET	6.0
1	A	16	ASP	5.2
1	B	228	PRO	5.0
1	B	235	VAL	4.9
1	B	83	ALA	4.8
1	B	234	THR	4.7
1	A	18	PRO	4.6
2	D	232	VAL	4.5
1	A	92	THR	4.5
1	F	48	ILE	4.5
1	A	234	THR	4.5
2	D	291	ALA	4.4
2	D	229	VAL	4.4
1	F	23	TYR	4.4
1	F	11	LEU	4.3
1	B	49	GLY	4.3
1	B	82	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	83	ALA	4.1
2	D	157	ASP	4.0
1	F	82	THR	4.0
1	E	17	GLY	4.0
1	F	75	ALA	3.9
2	D	84	ARG	3.8
1	B	75	ALA	3.7
1	F	10	ALA	3.7
1	A	150	PRO	3.6
1	B	24	VAL	3.6
1	F	228	PRO	3.6
1	A	154	ALA	3.5
1	C	121	ALA	3.5
1	F	68	LEU	3.4
1	A	108	THR	3.4
1	A	235	VAL	3.4
1	F	236	GLY	3.4
1	F	14	ILE	3.3
1	C	154	ALA	3.3
1	B	78	THR	3.2
1	A	93	TYR	3.2
1	E	83	ALA	3.2
1	B	12	ILE	3.2
1	C	23	TYR	3.2
1	B	94	ALA	3.2
1	A	228	PRO	3.2
1	B	80	THR	3.2
2	D	155	ASP	3.1
1	B	92	THR	3.1
2	D	92	THR	3.1
1	C	21	ALA	3.1
1	F	220	GLY	3.0
1	C	103	ASP	3.0
1	F	12	ILE	3.0
1	B	15	VAL	3.0
1	E	229	VAL	3.0
1	B	23	TYR	3.0
1	F	125	GLY	3.0
1	F	21	ALA	3.0
1	E	52	ALA	2.9
1	F	124	PRO	2.9
1	C	108	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	234	THR	2.9
2	D	234	THR	2.9
1	F	158	LEU	2.9
1	F	121	ALA	2.9
1	A	151	SER	2.9
1	F	130	ALA	2.9
1	B	96	ASP	2.8
2	D	108	ALA	2.8
1	F	290	GLY	2.8
1	F	210	ASP	2.8
1	A	232	VAL	2.8
1	F	1	MET	2.8
2	D	289	ALA	2.8
1	A	152	LEU	2.8
1	C	258	ASP	2.8
1	C	226	ALA	2.8
1	E	108	THR	2.8
1	B	14	ILE	2.8
2	D	95	PHE	2.8
1	C	15	VAL	2.8
2	D	154	ALA	2.8
1	A	83	ALA	2.7
1	E	234	THR	2.7
1	C	14	ILE	2.7
1	F	95	PHE	2.7
1	F	131	ALA	2.7
1	E	104	THR	2.7
2	D	102	PRO	2.7
1	F	289	ALA	2.7
1	B	74	THR	2.6
1	C	76	ASP	2.6
1	F	15	VAL	2.6
1	B	50	ARG	2.6
1	F	60	TYR	2.6
1	F	78	THR	2.6
1	F	72	SER	2.6
1	C	52	ALA	2.6
1	E	76	ASP	2.6
1	B	289	ALA	2.6
1	B	77	ARG	2.6
2	D	17	GLY	2.5
1	B	93	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	18	PRO	2.5
2	D	19	ASP	2.5
1	B	81	ALA	2.5
1	A	288	ARG	2.5
1	B	151	SER	2.5
1	B	60	TYR	2.5
2	D	93	TYR	2.5
1	E	258	ASP	2.5
1	A	95	PHE	2.5
1	B	95	PHE	2.5
2	D	290	GLY	2.4
1	B	2	ALA	2.4
1	A	153	SER	2.4
1	C	235	VAL	2.4
1	C	72	SER	2.4
1	E	235	VAL	2.4
1	F	24	VAL	2.4
1	E	210	ASP	2.4
1	F	93	TYR	2.4
1	C	290	GLY	2.4
1	E	226	ALA	2.4
1	F	46	THR	2.3
1	F	102	PRO	2.3
1	B	76	ASP	2.3
1	E	16	ASP	2.3
1	B	52	ALA	2.3
1	F	62	GLU	2.3
1	C	100	GLN	2.3
1	A	289	ALA	2.3
1	C	24	VAL	2.3
1	F	108	THR	2.3
1	B	227	GLN	2.3
1	B	102	PRO	2.3
2	D	258	ASP	2.3
1	C	59	GLU	2.2
1	C	98	GLU	2.2
1	F	79	PRO	2.2
1	E	19	ASP	2.2
1	A	149	ARG	2.2
1	C	291	ALA	2.2
1	F	80	THR	2.2
1	E	151	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	12	ILE	2.2
1	C	92	THR	2.2
1	C	95	PHE	2.2
1	B	63	SER	2.2
1	F	132	LEU	2.2
2	D	150	PRO	2.2
1	B	131	ALA	2.2
1	F	74	THR	2.2
1	F	153	SER	2.1
1	B	53	ARG	2.1
1	E	131	ALA	2.1
1	C	233	ASP	2.1
1	A	1	MET	2.1
2	D	103	ASP	2.1
1	B	101	ILE	2.1
1	B	58	ALA	2.1
1	A	19	ASP	2.1
1	B	72	SER	2.1
1	B	48	ILE	2.1
2	D	158	LEU	2.1
1	B	10	ALA	2.1
1	A	210	ASP	2.0
1	C	155	ASP	2.0
1	F	282	SER	2.0
1	E	152	LEU	2.0
2	D	228	PRO	2.0
1	E	268	VAL	2.0
1	F	66	VAL	2.0
2	D	235	VAL	2.0
1	B	17	GLY	2.0
1	B	51	ASP	2.0
1	E	102	PRO	2.0
2	D	156	PRO	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 monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
4	PO4	F	401	5/5	0.72	0.09	96,100,110,111	0
3	GOL	B	402	6/6	0.73	0.19	72,78,83,84	0
3	GOL	B	401	6/6	0.74	0.16	77,86,89,90	0
4	PO4	B	403	5/5	0.77	0.11	79,90,94,95	0
3	GOL	A	401	6/6	0.78	0.16	48,60,67,68	0
4	PO4	D	302	5/5	0.84	0.09	69,75,76,81	0
3	GOL	D	301	6/6	0.84	0.12	67,71,76,80	0
3	GOL	E	401	6/6	0.85	0.17	65,68,70,72	0
4	PO4	A	402	5/5	0.86	0.09	68,68,74,81	0
4	PO4	E	402	5/5	0.89	0.08	77,79,82,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.