



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6NS6
Title : Crystal structure of fungal lipoxygenase from *Fusarium graminearum*. P21 crystal form.
Authors : Pakhomova, S.; Boeglin, W.E.; Neau, D.B.; Bartlett, S.G.; Brash, A.R.; Newcomer, M.E.
Deposited on : 2019-01-24
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

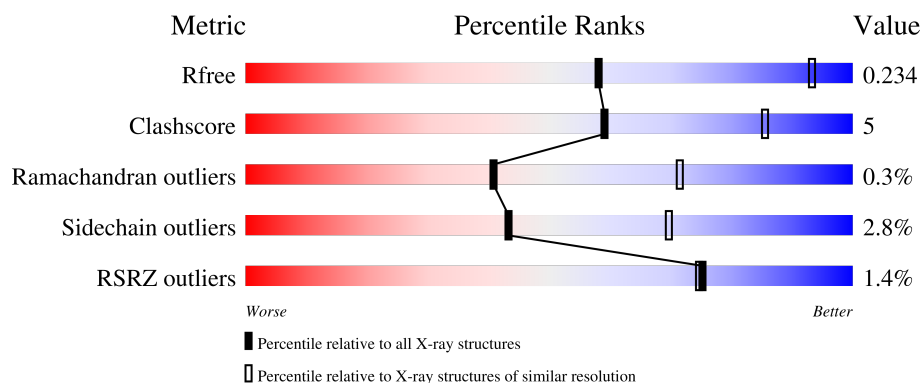
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	769	<div> <div></div> <div>75% 12% 13%</div> </div>
1	B	769	<div> <div></div> <div>73% 12% 14%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10538 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 lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5281	3382	880	1009	10			
1	B	664	Total	C	N	O	S	0	0	0
			5253	3362	874	1007	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP I1REW2
A	-22	GLY	-	expression tag	UNP I1REW2
A	-21	ARG	-	expression tag	UNP I1REW2
A	-20	ASP	-	expression tag	UNP I1REW2
A	-19	PRO	-	expression tag	UNP I1REW2
A	-18	ASN	-	expression tag	UNP I1REW2
A	-17	SER	-	expression tag	UNP I1REW2
A	-16	SER	-	expression tag	UNP I1REW2
A	-15	SER	-	expression tag	UNP I1REW2
A	-14	VAL	-	expression tag	UNP I1REW2
A	-13	ASP	-	expression tag	UNP I1REW2
A	-12	LYS	-	expression tag	UNP I1REW2
A	-11	LEU	-	expression tag	UNP I1REW2
A	-10	ALA	-	expression tag	UNP I1REW2
A	-9	ALA	-	expression tag	UNP I1REW2
A	-8	ALA	-	expression tag	UNP I1REW2
A	-7	LEU	-	expression tag	UNP I1REW2
A	-6	GLU	-	expression tag	UNP I1REW2
A	-5	HIS	-	expression tag	UNP I1REW2
A	-4	HIS	-	expression tag	UNP I1REW2
A	-3	HIS	-	expression tag	UNP I1REW2
A	-2	HIS	-	expression tag	UNP I1REW2
A	-1	HIS	-	expression tag	UNP I1REW2
A	0	HIS	-	expression tag	UNP I1REW2
B	-23	MET	-	expression tag	UNP I1REW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP I1REW2
B	-21	ARG	-	expression tag	UNP I1REW2
B	-20	ASP	-	expression tag	UNP I1REW2
B	-19	PRO	-	expression tag	UNP I1REW2
B	-18	ASN	-	expression tag	UNP I1REW2
B	-17	SER	-	expression tag	UNP I1REW2
B	-16	SER	-	expression tag	UNP I1REW2
B	-15	SER	-	expression tag	UNP I1REW2
B	-14	VAL	-	expression tag	UNP I1REW2
B	-13	ASP	-	expression tag	UNP I1REW2
B	-12	LYS	-	expression tag	UNP I1REW2
B	-11	LEU	-	expression tag	UNP I1REW2
B	-10	ALA	-	expression tag	UNP I1REW2
B	-9	ALA	-	expression tag	UNP I1REW2
B	-8	ALA	-	expression tag	UNP I1REW2
B	-7	LEU	-	expression tag	UNP I1REW2
B	-6	GLU	-	expression tag	UNP I1REW2
B	-5	HIS	-	expression tag	UNP I1REW2
B	-4	HIS	-	expression tag	UNP I1REW2
B	-3	HIS	-	expression tag	UNP I1REW2
B	-2	HIS	-	expression tag	UNP I1REW2
B	-1	HIS	-	expression tag	UNP I1REW2
B	0	HIS	-	expression tag	UNP I1REW2


- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

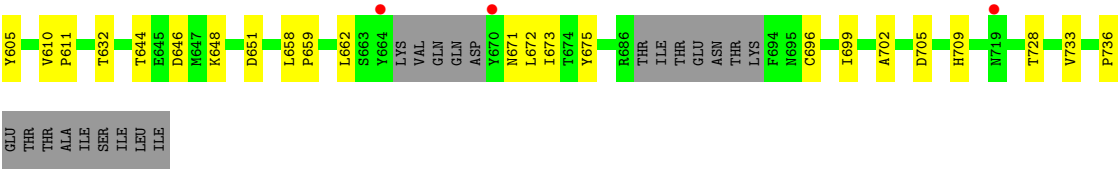
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0

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.

- Chain A: 
- 75% 12% 13%
- Met GLY ARG ASP PRO ASN SER SER SER VAL ASN LYS LEU ALA LEU GLU HIS HIS HIS HIS MET SER SER VAL VAL VAL V9 L19 E33 V34 W35 M42 L45 N56 G57 T58 L59 L69 L79 F105 P106 L111 D122
- D125 H130 D134 G135 A136 A137 A138 A139 A140 A141 A142 A143 A144 A145 A146 A147 A148 A149 A150 A151 A152 A153 A154 A155 A156 A157 A158 A159 A160 A161 A162 A163 A164 A165 A166 A167 A168 A169 A170 A171 A172 A173 A174 A175 A176 A177 A178 A179 A180 A181 A182 A183 A184 A185 A186 A187 A188 A189 A190 A191 A192 A193 A194 A195 A196 A197 A198 A199 A200 A201 A202 A203 A204 A205 A206 A207 A208 A209 A210 A211 A212 A213 A214 A215 A216 A217 A218 A219 A220 A221 A222 A223 A224 A225 A226 A227 A228 A229 A230 A231 A232 A233 A234 A235 A236 A237 A238 A239 A240 A241 A242 A243 A244 A245 A246 A247 A248 A249 A250 A251 A252 A253 A254 A255 A256 A257 A258 A259 A260 A261 A262 A263 A264 A265 A266 A267 A268 A269 A270 A271 A272 A273 A274 A275 A276 A277 A278 A279 A280 A281 A282 A283 A284 A285 A286 A287 A288 A289 A290 A291 A292 A293 A294 A295 A296 A297 A298 A299 A300 A301 A302 A303 A304 A305 A306 A307 A308 A309 A310 A311 A312 A313 A314 A315 A316 A317 A318 A319 A320 A321 A322 A323 A324 A325 A326 A327 A328 A329 A330 A331 A332 A333 A334 A335 A336 A337 A338 A339 A340 A341 A342 A343 A344 A345 A346 A347 A348 A349 A350 A351 A352 A353 A354 A355 A356 A357 A358 A359 A360 A361 A362 A363 A364 A365 A366 A367 A368 A369 A370 A371 A372 A373 A374 A375 A376 A377 A378 A379 A380 A381 A382 A383 A384 A385 A386 A387 A388 A389 A390 A391 A392 A393 A394 A395 A396 A397 A398 A399 A400 A401 A402 A403 A404 A405 A406 A407 A408 A409 A410 A411 A412 A413 A414 A415 A416 A417 A418 A419 A420 A421 A422 A423 A424 A425 A426 A427 A428 A429 A430 A431 A432 A433 A434 A435 A436 A437 A438 A439 A440 A441 A442 A443 A444 A445 A446 A447 A448 A449 A450 A451 A452 A453 A454 A455 A456 A457 A458 A459 A460 A461 A462 A463 A464 A465 A466 A467 A468 A469 A470 A471 A472 A473 A474 A475 A476 A477 A478 A479 A480 A481 A482 A483 A484 A485 A486 A487 A488 A489 A490 A491 A492 A493 A494 A495 A496 A497 A498 A499 A500 A501 A502 A503 A504 A505 A506 A507 A508 A509 A510 A511 A512 A513 A514 A515 A516 A517 A518 A519 A520 A521 A522 A523 A524 A525 A526 A527 A528 A529 A530 A531 A532 A533 A534 A535 A536 A537 A538 A539 A540 A541 A542 A543 A544 A545 A546 A547 A548 A549 A550 A551 A552 A553 A554 A555 A556 A557 A558 A559 A560 A561 A562 A563 A564 A565 A566 A567 A568 A569 A570 A571 A572 A573 A574 A575 A576 A577 A578 A579 A580 A581 A582 A583 A584 A585 A586 A587 A588 A589 A590 A591 A592 A593 A594 A595 A596 A597 A598 A599 A600 A601 A602 A603 A604 A605 A606 A607 A608 A609 A610 A611 A612 A613 A614 A615 A616 A617 A618 A619 A620 A621 A622 A623 A624 A625 A626 A627 A628 A629 A630 A631 A632 A633 A634 A635 A636 A637 A638 A639 A640 A641 A642 A643 A644 A645 A646 A647 A648 A649 A650 A651 A652 A653 A654 A655 A656 A657 A658 A659 A660 A661 A662 A663 A664 A665 A666 A667 A668 A669 A670 A671 A672 A673 A674 A675 A676 A677 A678 A679 A680 A681 A682 A683 A684 A685 A686 A687 A688 A689 A690 A691 A692 A693 A694 A695 A696 A697 A698 A699 A700 A701 A702 A703 A704 A705 A706 A707 A708 A709 A710 A711 A712 A713 A714 A715 A716 A717 A718 A719 A720 A721 A722 A723 A724 A725 A726 A727 A728 A729 A730 A731 A732 A733 A734 A735 A736 A737 A738 A739 A740 A741 A742 A743 A744 A745 A746 A747 A748 A749 A750 A751 A752 A753 A754 A755 A756 A757 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A772 A773 A774 A775 A776 A777 A778 A779 A780 A781 A782 A783 A784 A785 A786 A787 A788 A789 A790 A791 A792 A793 A794 A795 A796 A797 A798 A799 A800 A801 A802 A803 A804 A805 A806 A807 A808 A809 A810 A811 A812 A813 A814 A815 A816 A817 A818 A819 A820 A821 A822 A823 A824 A825 A826 A827 A828 A829 A830 A831 A832 A833 A834 A835 A836 A837 A838 A839 A840 A841 A842 A843 A844 A845 A846 A847 A848 A849 A850 A851 A852 A853 A854 A855 A856 A857 A858 A859 A860 A861 A862 A863 A864 A865 A866 A867 A868 A869 A870 A871 A872 A873 A874 A875 A876 A877 A878 A879 A880 A881 A882 A883 A884 A885 A886 A887 A888 A889 A890 A891 A892 A893 A894 A895 A896 A897 A898 A899 A900 A901 A902 A903 A904 A905 A906 A907 A908 A909 A910 A911 A912 A913 A914 A915 A916 A917 A918 A919 A920 A921 A922 A923 A924 A925 A926 A927 A928 A929 A930 A931 A932 A933 A934 A935 A936 A937 A938 A939 A940 A941 A942 A943 A944 A945 A946 A947 A948 A949 A950 A951 A952 A953 A954 A955 A956 A957 A958 A959 A960 A961 A962 A963 A964 A965 A966 A967 A968 A969 A970 A971 A972 A973 A974 A975 A976 A977 A978 A979 A980 A981 A982 A983 A984 A985 A986 A987 A988 A989 A990 A991 A992 A993 A994 A995 A996 A997 A998 A999 A1000 A1001 A1002 A1003 A1004 A1005 A1006 A1007 A1008 A1009 A1010 A1011 A1012 A1013 A1014 A1015 A1016 A1017 A1018 A1019 A1020 A1021 A1022 A1023 A1024 A1025 A1026 A1027 A1028 A1029 A1030 A1031 A1032 A1033 A1034 A1035 A1036 A1037 A1038 A1039 A1040 A1041 A1042 A1043 A1044 A1045 A1046 A1047 A1048 A1049 A1050 A1051 A1052 A1053 A1054 A1055 A1056 A1057 A1058 A1059 A1060 A1061 A1062 A1063 A1064 A1065 A1066 A1067 A1068 A1069 A1070 A1071 A1072 A1073 A1074 A1075 A1076 A1077 A1078 A1079 A1080 A1081 A1082 A1083 A1084 A1085 A1086 A1087 A1088 A1089 A1090 A1091 A1

- Chain B:
-
- | Amino Acid | Frequency (%) |
|-------------------|---------------|
| MET | ~73% |
| VAL | ~12% |
| LYS | ~14% |
| Other Amino Acids | < 1% |



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.01Å 94.77Å 105.08Å 90.00° 106.16° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 39.26 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-3.30) 99.5 (39.26-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.194 , 0.241 0.194 , 0.234	Depositor DCC
R_{free} test set	664 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	100.4	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10538	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/5410	0.69	0/7351
1	B	0.62	0/5381	0.69	0/7314
All	All	0.62	0/10791	0.69	0/14665

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5281	0	5168	46	0
1	B	5253	0	5125	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	10538	0	10293	97	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 5.

The worst 5 of 97 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:454:LEU:CD2	1:B:662:LEU:HD21	2.15	0.77
1:B:454:LEU:HD21	1:B:662:LEU:HD21	1.80	0.63
1:B:300:ARG:NH2	1:B:309:GLN:O	2.37	0.58
1:B:125:ASP:OD1	1:B:130:HIS:NE2	2.33	0.57
1:A:504:ARG:NH2	1:A:519:TYR:OH	2.35	0.57

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	656/769 (85%)	602 (92%)	52 (8%)	2 (0%)	41	71
1	B	654/769 (85%)	602 (92%)	50 (8%)	2 (0%)	41	71
All	All	1310/1538 (85%)	1204 (92%)	102 (8%)	4 (0%)	41	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	SER
1	B	593	SER
1	A	442	ARG
1	B	453	LEU

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	566/660 (86%)	552 (98%)	14 (2%)	47	72
1	B	562/660 (85%)	544 (97%)	18 (3%)	39	67
All	All	1128/1320 (86%)	1096 (97%)	32 (3%)	43	70

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	651	ASP
1	B	671	ASN
1	A	696	CYS
1	A	671	ASN
1	B	696	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	590	HIS
1	B	709	HIS
1	B	719	ASN
1	B	629	GLN
1	A	629	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	666/769 (86%)	-0.19	8 (1%) 79 78	76, 120, 163, 187	0
1	B	664/769 (86%)	-0.17	11 (1%) 70 68	73, 119, 161, 196	0
All	All	1330/1538 (86%)	-0.18	19 (1%) 75 75	73, 119, 163, 196	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	LEU	3.9
1	A	58	THR	3.2
1	B	318	LEU	3.1
1	B	59	LEU	3.1
1	B	320	GLY	2.8

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
2	FE2	A	801	1/1	0.98	0.15	97,97,97,97	0
2	FE2	B	801	1/1	0.98	0.14	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.